ERDC/EL TR-02-27

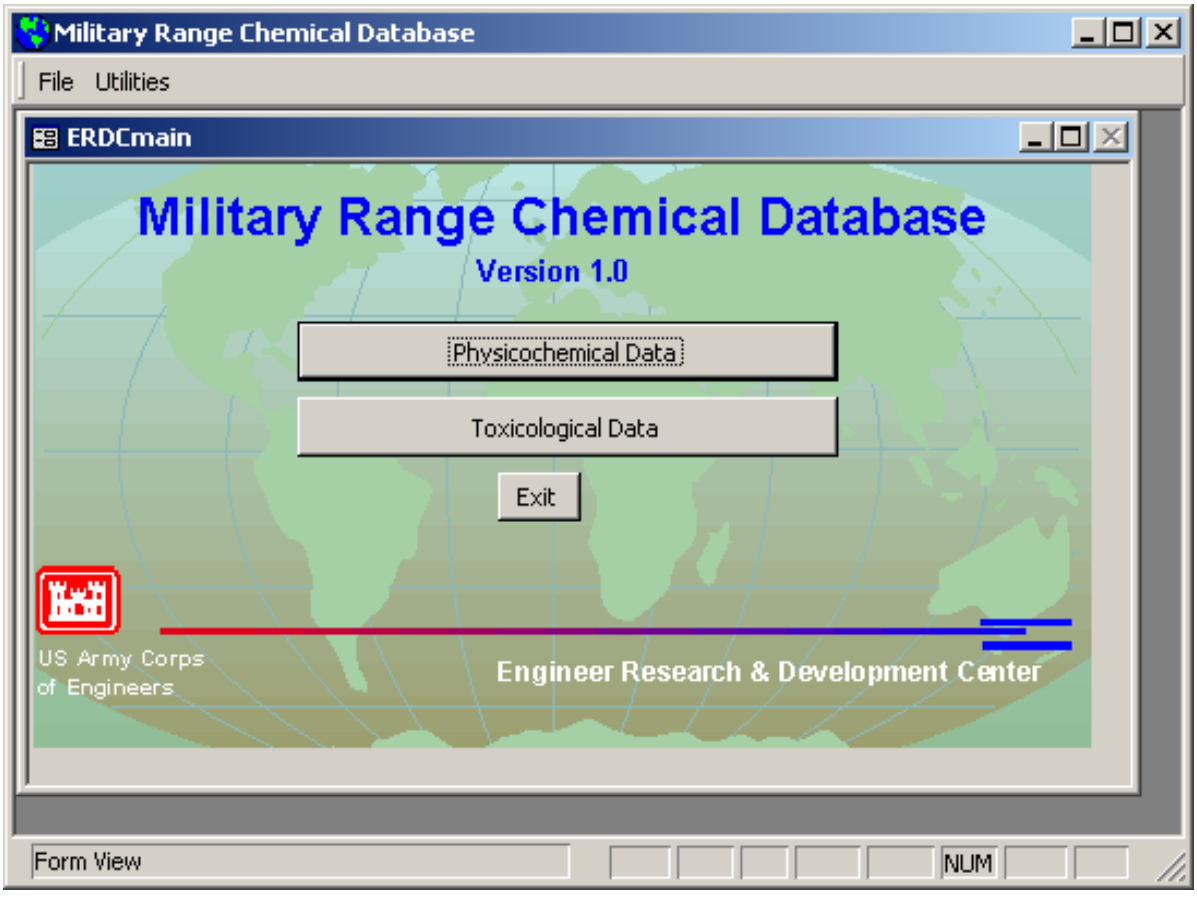
US Army Corps
of Engineers®
Engineer Research and
Development Center

Compilation of Physical and Chemical Properties and Toxicity Benchmarks for Military Range Compounds

Mansour Zakikhani, Mark S. Dortch,
and Jeffrey A. Gerald

September 2002

Note: Appendix B has been modified from the version in the printed report, dated September 2002.



Environmental Laboratory

ERDC/EL TR-02-27
September 2002

Compilation of Physical and Chemical Properties and Toxicity Benchmarks for Military Range Compounds

by Mansour Zakikhani, Mark S. Dortch, Jeffrey A. Gerald

Environmental Laboratory
U.S. Army Engineer Research and Development Center
3909 Halls Ferry Road
Vicksburg, MS 39180-6199

Final report

Prepared for U.S. Army Environmental Center
Aberdeen Proving Ground, MD 21010-5401

Contents

List of Figures

List of Tables

Preface

The purpose of this report is to describe the development of a database of physicochemical properties of selected chemicals of interest to the U.S. Army. In addition to collection of physicochemical properties described herein, toxicity benchmarks for range chemicals (Appendix B) were compiled under this project by the U.S. Army Center for Health Promotion and Preventive Medicine (CHPPM). The U.S. Army Environmental Center (USAEC), Aberdeen Proving Ground, Maryland, sponsored this work. Dr. Ira May was the Project Monitor, and Ms. Tamera L. Rush, USAEC/Booz Allen Hamilton, was the project coordinator.

Drs. Mansour Zakikhani and Mark S. Dortch and Mr. Jeffrey A. Gerald, Water Quality and Contaminant Modeling Branch (WQCMB), Environmental Processes and Engineering Division (EPED), Environmental Laboratory (EL), Vicksburg, MS, U.S. Army Engineer Research and Development Center (ERDC), prepared this report. Appendix B was prepared by Mr. Christopher Salice and Drs. Howard T. Bausum and Mark S. Johnson of CHPPM. This work was conducted under the general supervision of Dr. Dortch, Chief, WQCMB, Dr. Richard E. Price, Chief, EPED, and Dr. Edwin A. Theriot, Director, EL.

The authors would like to thank the following individuals for their valuable help: Dr. Herbert Fredickson of EPED and Mr. John S. Furey, DYNCORP, who gathered the half-life data provided in Appendix A and chemical grouping in Chapter 1, and Dr. Fredrick Gary Dolislager from the University of Tennessee, Department of Ecology and Evolutionary Biology, Knoxville, TN, who provided missing references for the RAIS database.

Mr. Christian J. McGrath and Dr. Carlos E. Ruiz, WQCMB, reviewed this report. Ms. Rush provided additional comments and suggestions.

At the time of publication of this report, Dr. James R. Houston was Director of ERDC, and COL John W. Morris III, EN, was Commander and Executive Director.

This report should be cited as follows:

> Zakikhani, M., Dortch, M. S., and Gerald, J. A. (2002). "Compilation of physical and chemical properties and toxicity benchmarks for military range compounds," ERDC/EL TR-02-27, U.S. Army Engineer Research and Development Center, Vicksburg, MS.

1 Introduction

Background

The U.S. Army Environmental Center (USAEC) has developed a test program to identify and quantify the emissions that result from weapons firing and from the use of pyrotechnic devices. The test program is divided into three distinct areas: characterization of smoke and pyrotechnic emissions, a firing point emission study, and an exploding ordnance emission study. One of the tasks associated with this program was to develop a database of physicochemical properties for the chemicals of greatest concern to USAEC.

A wide variety of physical and chemical data is essential to understand the fate and impact of chemicals released into the environment, to develop strategies for the removal or destruction of harmful byproducts, or to design processes and products that minimize environmental impact. Ideally, these data would be most useful if compiled into a single, internally consistent database, which was the goal of this effort. The database currently includes 11 priority physical and chemical properties (Zakikhani et al. 2001) and toxicological benchmark data developed by the U.S. Army Center for Health Promotion and Preventive Maintenance (CHPPM).

Physicochemical properties of chemicals are needed as input to fate and transport models used to predict the extent and behavior of contaminant plumes in various media (soil, air, water, ecosystems). The data also are needed for exposure and risk assessment characterization. For example, the Army Risk Assessment Modeling System (ARAMS) is a computer-based decision support system that integrates multimedia fate/transport, exposure, intake/uptake, and effect of military relevant compounds, explosives, and depleted uranium to assess human and ecological probabilistic risks (*http://www.wes.army.mil/el/arams/arams.html*). Toxicological benchmark data are required for effects assessment in risk characterization.

The majority of chemicals listed in the database are the original constituents of munitions as well as emissions, which are generated during use. Table 1 shows examples of range compounds for high explosives and smokes and obscurants available in the database. For each chemical, primary properties that affect fate/transport of chemicals in the environment were gathered and added to the database. Typical properties required for fate and transport modeling are shown in Table 2. Some properties can be estimated from other available

Table 1
Examples of Range Compounds

High Explosives Compounds
•2,4,6-trinitrotoluene (TNT) •2-Amino-4,6-Dinitrotoluene (2ADNT) •4-Amino-2,6-Dinitrotoluene (4ADNT) •1,3,5-Trinitrobenzene (1,3,5TNB) •1,3-Dinitrobenzene (1,3DNB) •Hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX) •Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX) •N,2,4,6-Tetranitro-N-methylaniline (Tetryl) •1,2,3-Propanetriol trinitrate (Nitroglycerine) •Pentaerythritol tetranitrate (PETN)
Examples of Database Chemicals Associated with Military Smokes and Obscurants
•1,4-diaminoanthraquinone (DAA) •Dibenzochrysenedione (vat Yellow DBC) •1,4- diamino-2,3-dihydroanthraquinone •1,4-diamino-2-(2-quinolyl)-1,3-indandione •1,4-di-p-toluidino-9,10-anthraquinone •2-(2-quinolyl)-1,3-indandione •1-(methylamino)-9,10-anthracenedione

Table 2
Typical Chemical-Specific Properties Required for Fate/Transport Modeling

Parameter	**Units**
Molecular weight	g/mole
Henry's Law Constant	atm m^3/mole
Octanol-water partitioning coefficient for organics	mL/g
Distribution coefficient for partitioning to solids for nonorganics	mL/g
Water solubility	mg/L
Half-life in air	days
Half-life in soil	days
Half-life in surface water	days
Half-life in aerobic groundwater	days
Half-life in anoxic groundwater	days
Molecular diffusivity in water	cm^2/sec

properties, such as molecular diffusivity. Others, such as the distribution coefficient for inorganics, may depend on media-specific data. Other properties can be required depending on the details of the reaction pathways considered, e.g., whether oxidation-reduction, photolysis, and biodegradation reactions are considered as reaction paths rather than being described as lumped pseudo-first-order decay (half-life). For many military unique or relevant compounds, detailed process information will not be available. Thus, lumped process decay will usually be the approach. Additionally, for explosives-related compounds,

decay in soil and groundwater is dependent on local conditions (e.g., redox). The local and site-specific conditions that may affect the properties are not provided in the database.

Objective

The objective of this project was to identify available data on physical and chemical properties required for fate and transport modeling of chemicals typically associated with munitions and their respective emissions and to compile these data as well as associated toxicity benchmarks.

Scope of Work

This section describes the steps that were taken to develop the database of physicochemical properties for chemical compounds listed by USAEC (Table 3). The sources and references of the physicochemical data are provided. The data gaps and available software for estimation of properties are described. The database was developed using Microsoft Access 2000 software. A copy of the database is included on a CD accompanying this report. Additional data on half-life values were collected (Appendix A), but because of significant missing data values, these data were not included in the database. However, there are other half-life data that were included in the database. Benchmark toxicological data developed under this project by CHPPM are given in Appendix B.

The USAEC chemicals were grouped into ten classes or groups (Table 3): halogenated hydrocarbons, nonhalogenated hydrocarbons, explosives, polycyclic aromatic hydrocarbons (PAHs) + polychlorinated biphenyls (PCBs), alcohols/ketones, biocides/dyes, metals/inorganics, gases, furans+dioxins, and other. This grouping is one of several ways that chemicals can be grouped.

The physicochemical properties were obtained from a variety of sources (Chapter 2). For many of the chemicals on the USAEC list, sufficient data on some of the physicochemical properties could not be obtained. For these chemicals, the physicochemical properties may be estimated from other sources such as the U.S. Environmental Protection Agency's (USEPA) ASTER (ASsessment Tools for the Evaluation of Risk program), http://www.epa.gov/med/databases/aster.htm, or other estimation software described in Chapter 2.

The report is divided into six chapters and three appendixes. Chapter 2 describes the sources of data included in the database and discusses data gaps. Chapter 3 explains the structure used in the database. Chapter 4 provides information about user interface and options of the database. Chapter 5 gives results and analysis of identifying data gaps and estimation techniques. Chapter 6 summarizes the study and provides conclusions and offers recommendations for future work. Appendix C is a glossary of physicochemical properties.

Table 3
List of USAEC Priority Chemicals

ID	Chemical Name	CAS Number	Formula	Group
1	1,2-Dichloroethene (cis)	156-59-2	C2H2Cl2	halogenated
2	1,2-Dichloroethene (trans)	156-60-5	C2H2Cl2	halogenated
3	(1,2-dichloroethyl) benzene	1074-11-9	C8H8Cl2	halogenated
4	1,2,4-Trimethylbenzene	95-63-6	C9H12	hydrocarbons
5	1,2-Dichlorethane	107-06-2	C2H4Cl2	halogenated
6	1,2-Dichloro-3-methylbenzene	32768-54-0	C7H6Cl2	halogenated
7	1,2-Dichloroethene (cis/trans MIXTURE)	540-59-0	C2H2Cl2	halogenated
8	1,3,5-Trimethylbenzene (MESITYLENE)	108-67-8	C9H12	hydrocarbons
9	1,3,5-Trinitrobenzene	99-35-4	C6H3N3O6	explosives
10	1,3-Butadiene	106-99-0	C4H6	hydrocarbons
11	1,3-Dinitrobenzene	99-65-0	C6H4N2O4	explosives
12	1,4-Diamino-2,3-dihydroanthraquinone (DDA) violet-dye mix	81-63-0	C14H12N2O2	biocides/dyes
13	1,4-Di-p-toluidinoanthraquinone (PTA) Green 3	128-80-3	C28H22N2O2	biocides/dyes
14	1-Butanol	71-36-3	C4H10O	alcohols/ketones
15	1-Butene	106-98-9	C4H8	hydrocarbons
16	Isobutylene	115-11-7	C4H8	hydrocarbons
17	1-Chloro-2-methylbenzene	95-49-8	C7H7Cl	halogenated
18	1-Chloro-3-methylbenzene	108-41-8	C7H7Cl	halogenated
19	1-Hexene	592-41-6	C6H12	hydrocarbons
20	1-Pentene	109-67-1	C5H10	hydrocarbons
21	1-(Methylamino)anthraquinone (Disperse Red 9)	82-38-2	C15H11NO2	biocides/dyes
22	2-(2-quinolinyl)-1H-indene-1,3-(2H)-dione	8003-22-3	C18H11NO2	biocides/dyes
23	2-(2-quinolinyl)-1,3-indandione (D & C yellow no. 11)	8003-22-3	C18H11NO2	biocides/dyes
24	2,3-Butanedione	625-34-3	C4H6O2	alcohols/ketones
25	2,3,7,8-Tetrachlorodibenzo-p-Dioxin	1746-01-6	C12H4Cl4O2	furans+dioxins
26	2,4,6-Trinitrotoluene (TNT)	118-96-7	C7H5N3O6	explosives
27	2,4-Dinitrotoluene (DNT; 2,4-DNT)	121-14-2	C7H6N2O4	explosives
28	2,6-Dinitrotoluene (2,6-DNT)	606-20-2	C7H6N2O4	explosives
29	2,5-Dimethylfuran	625-86-5	C6H8O	furans+dioxins

(Sheet 1 of 6)

* = Unknown CAS (chemical abstract service) or Registry Number, or incorrect chemical name.

Table 3 (Continued)

ID	Chemical Name	CAS Number	Formula	Group
30	2-Amino-4,6-Dinitrotoluene	35572-78-2	C7H7N3O4	explosives
31	2-amino-9,10-anthracenedione (AAQ)	117-79-3	C14H9NO2	biocides/dyes
32	2-Butanone	78-93-3	C4H8O	alcohols/ketones
33	2-Furaldehyde	98-01-1	C5H4O2	alcohols/ketones
34	2-Heptanone	110-43-0	C7H14O	alcohols/ketones
35	2-Methyl-1-butene	563-46-2	C5H10	hydrocarbons
36	2-Methylfuran	534-22-5	C5H6O	furans+dioxins
37	2-Methylthiophene	554-14-3	C5H6S	hydrocarbons
38	2-Nitrotoluene (ONT)	88-72-2	C7H7NO2	explosives
39	2-Pentanone	107-87-9	C5H10O	alcohols/ketones
40	2-Propanol	67-63-0	C3H8O	alcohols/ketones
41	2-Thiophenecarboxaldehyde	98-03-3	C5H4OS	alcohols/ketones
42*	**3-(phenylhydrazone)-1H-Indole-2,3-dione***			
43	3-Furaldehyde	498-60-2	C5H4O2	alcohols/ketones
44	3-Methyl-1-butene	563-45-1	C5H10	hydrocarbons
45	3-Methylfuran	930-27-8	C5H6O	furans+dioxins
46	3-Methylthiophene	616-44-4	C5H6S	hydrocarbons
47	3-Nitrotoluene	99-08-1	C7H7NO2	explosives
48*	**4-1,2,4-oxadizaolin-3-one-2,5-diphenyl-delta***			
49	4-Amino-2,6-Dinitrotoluene (4ADNT)	19406-51-0	C7H7N3O4	explosives
50	4-Ethyltoluene	622-96-8	C9H12	hydrocarbons
51	4-Methyl-2-Pentanone	108-10-1	C6H12O	alcohols/ketones
52	4-Nitrotoluene	99-99-0	C7H7NO2	explosives
53	4-phenoxy-2(1H)-quinolinone	66662-28-0	C15H11N1O2	biocides/dyes
54	Acenaphthene	83-32-9	C12H10	PAHs+PCBs
55	Acenaphthylene	208-96-8	C12H8	PAHs+PCBs
56	Acetaldehyde	75-07-0	C2H4O	alcohols/ketones
57	Acetic Acid	64-19-7	C2H4O2	other
58	Acetone	67-64-1	C3H6O	alcohols/ketones
59	Acetonitrile	75-05-8	C2H3N	hydrocarbons
60	Acetophenone	98-86-2	C8H8O	alcohols/ketones
61	Acetylene	74-86-2	C2H2	hydrocarbons
62	Acrolein	107-02-8	C3H4O	hydrocarbons
63	Acrylonitrile	107-13-1	C3H3N	hydrocarbons

(Sheet 2 of 6)

Table 3 (Continued)

ID	Chemical Name	CAS Number	Formula	Group
64	Aluminum	7429-90-5	Al	metals/inorganics
65	Anthracene	120-12-7	C14H10	PAHs+PCBs
66	Antimony	7440-36-0	Sb	metals/inorganics
67	Arsenic	7440-38-2	As	metals/inorganics
68	Barium	7440-39-3	Ba	metals/inorganics
69	Benzaldehyde	100-52-7	C7H6O	alcohols/ketones
70	Benzanthrone	82-05-3	C17H10O	biocides/dyes
71	Benzene	71-43-2	C6H6	hydrocarbons
72	Benzo(a)anthracene	56-55-3	C18H12	PAHs+PCBs
73	Benzo(a)pyrene	50-32-8	C20H12	PAHS+PCBs
74	Benzo(b)fluoranthene	205-99-2	C20H12	PAHS+PCBs
75	Benzo(e)pyrene	192-97-2	C20H12	PAHS+PCBs
76	Benzo(g,h,i)perylene	191-24-2	C22H12	PAHS+PCBs
77	Benzo(k)fluoranthene	207-08-9	C20H12	PAHS+PCBs
78	Benzofuran	271-89-6	C8H6O	furans+dioxins
79	Benzonitrile	100-47-0	C7H5N	Biocides/dyes
80	Beryllium	7440-41-7	Be	metals/inorganics
81	Bis(2-ethylhexyl)phthalate	117-81-7	C24H38O4	hydrocarbons
82	Butanal	123-72-8	C4H8O	alcohols/ketones
83	Cadmium	7440-43-9	Cd	metals/inorganics
84	Calcium	7440-70-2	Ca	metals/inorganics
85	Carbon Dioxide	124-38-9	CO2	gases
86	Carbon Disulfide	75-15-0	CS2	gases
87	Carbon Monoxide	630-08-0	CO	gases
88	Carbon Tetrachloride	56-23-5	CCl4	halogenated
89	Carbonyl Sulfide	463-58-1	COS	gases
90	Chlorobenzene	108-90-7	C6H5Cl	halogenated
91	Chloroethene (Vinyl chloride)	75-01-4	C2H3Cl	halogenated
92	Chloroform	67-66-3	CHCl3	halogenated
93	Chloromethane	74-87-3	CH3Cl	halogenated
94	Chromium	7440-47-3	Cr	metals/inorganics
95	Chrysene	218-01-9	C18H12	PAHs+PCBs
96	cis-2-Butene	590-18-1	C4H8	hydrocarbons
97	Cl2	7782-50-5	Cl2	gases
98	Cobalt	7440-48-4	Co	metals/inorganics
99	Copper	7440-50-8	Cu	metals/inorganics

(Sheet 3 of 6)

Table 3 (Continued)

ID	Chemical Name	CAS Number	Formula	Group
100	Dibenz(a,h)anthracene	53-70-3	C22H14	PAHs+PCBs
101	Dibenzo(b,def)chrysene-7,14 dione (C.I. vat yellow 4)	128-66-5	C24H12O2	biocides/dyes
102	Dibutyl phthalate	84-74-2	C16H22O4	hydrocarbons
103	Dichloroacetonitrile	3018-12-0	C2HCl2N	halogenated
104	Dichlorodiflouromethane	75-71-8	CCl2F2	halgenated
105	Dimethyltrisulfide	3658-80-8	C2H6S3	gases
106	Dioctyl phthalate	117-81-7	C24H38O4	other
107	Dioxin TEQ	1746-01-6	C12H4Cl4O2	furans+dioxins
108	Diphenylamine	122-39-4	C12H11N	biocides/dyes
109	Ethane	74-84-0	C2H6	hydrocarbones
110	Ethanol	64-17-5	C2H6O	Alcohols/ketones
111	Ethylbenzene	100-41-4	C8H10	hydrocarbons
112	Ethylchloride	75-00-3	C2H5Cl	halogenated
113	Ethylene	74-85-1	C2H4	hydrocarbons
114	Fluoranthene	206-44-0	C16H10	PAHs+PCBs
115	Fluorene	86-73-7	C13H10	PAHs+PCBs
116	Formaldehyde	50-00-0	CH2O	alcohols/ketones
117	Furan	110-00-9	C4H4O	furans+dioxins
118	HCl	7647-01-0	ClH	other
119	Heptanal	111-71-7	C7H14O	alcohols/ketones
120	Hexachlorobenzene	118-74-1	C6Cl6	halogenated
121	Hexachlorobutadiene	87-68-3	C4Cl6	halogenated
122	Hexachlorocyclopentadiene	77-47-4	C5Cl6	halogenated
123	Hexachloroethane	67-72-1	C2Cl6	halogenated
124	Hexanal	66-25-1	C6H12O	alcohols/ketones
125	Hexane	110-54-3	C6H14	other
126	HMX	2691-41-0	C4H8N8O8	explosives
127	Hydrogen Cyanide	74-90-8	CHN	biocides/dyes
128	i-Butane (isobutane)	75-28-5	C4H10	hydrocarbons
129	i-Butene (isobutene/E-butylene)	115-11-7	C4H8	hydrocarbons
130	Indeno(1,2,3-cd)pyrene	193-39-5	C22H12	PAHs+PCBs
131	Isothiocyanatomethane	556-61-6	C2H3NS	biocides/dyes
132	Lead	7439-92-1	Pb	Metals/inorganics
133	Xylene (mixed isomers)	1330-20-7	C24H30	hydrocarbons
134	m-Xylene (meta-xylene)	108-38-3	C8H10	hydrocarbons
135	p-Xylene (para-xylene)	106-42-3	C8H10	hydrocarbons

(Sheet 4 of 6)

Table 3 (Continued)

ID	Chemical Name	CAS Number	Formula	Group
136	Magnesium	7439-95-4	Mg	metals/inorganics
137	Manganese	7439-96-5	Mn	metals/inorganics
138	m-Dichlorobenzene	541-73-1	C6H4Cl2	hydrocarbons
139	Mercury	7439-97-6	Hg	metals/inorganics
140	Methacrolein	78-85-3	C4H6O	alcohols/ketons
141	Methane	74-82-8	CH4	hydrocarbons
142	Methylene Chloride	75-09-2	CH2Cl2	halogenated
143	Methylnitrite	624-91-9	CH3NO2	explosives
144	Methyl-t-butylether (MTBE)	1634-04-4	C5H12O	alcohols/ketons
145	Methyl-vinyl ketone	78-94-4	C4H6O	alcohols/ketons
146	Naphthalene	91-20-3	C10H8	PAHs+PCBs
147	n-Butane	106-97-8	C4H10	hydrocarbons
148	n-Decane	124-18-5	C10H22	hydrocarbons
149	NH3 (Ammonia)	7664-41-7	H3N	gases
150	n-Hexane	110-54-3	C6H14	hydrocarbons
151	Nickel	7440-02-0	Ni	metals/inorganics
152	Nitric Acid	7697-37-2	HNO3	other
153	Nitrobenzene	98-95-3	C6H5NO2	explosives
154	Nitrogen Oxide (NOx)	10102-44-0	NO2*	gases
155	Nitroglycerine	55-63-0	C3H5N3O9	explosives
156	Nitromethane	75-52-5	CH3NO2	explosives
157	Nonanal	124-19-6	C9H18O	alcohols/ketons
158	OCDD (1,2,3,4,6,7,8,9-OCDD)	3268-87-9	C12Cl8O2	furans+dioxins
159	Octanal	124-13-0	C8H16O	alcohols/ketons
160	o-Dichlorobenzene	95-50-1	C6H4Cl2	halogenated
161	o-methoxy-phenyl-azo-b-naphthol (Oil Red G)	1229-55-6	C17H14N2O2	biocides/dyes
162	o-Xylene (ortho-xylene)	95-47-6	C8H10	hydrocarbons
163	Particulate Cyanide	57-12-5	CN--	inorganics
164	p-Dichlorobenzene (para-Dichlorobenzene)	106-46-7	C6H4Cl2	halogenated
165	Pentaerythritoltetranitrate (PETN)	78-11-5	C5H8N4O12	explosives
166	Perchloroethylene	127-18-4	C2Cl4	halogenated
167	Phenanthrene	85-01-8	C14H10	PAHs+PCBs
168	Phenol	108-95-2	C6H6O	alcohols/ketons
169	Phenylacetylene (Ethynyl benzene)	536-74-3	C8H6	hydrocarbons
170	Phosphorus	7723-14-0	P	other

(Sheet 5 of 6)

Table 3 (Concluded)

ID	Chemical Name	CAS Number	Formula	Group
171	Propanal	123-38-6	C3H6O	alcohols/ketones
172	Propane	74-98-6	C3H8	hydrocarbons
173	Propene	115-07-1	C3H6	hydrocarbons
174	Propylene	115-07-1	C3H6	hydrocarbons
175	Propyne	74-99-7	C3H4	hydrocarbons
176	Pyrene	129-00-0	C16H10	PAHs+PCBs
177	RDX	121-82-4	C3H6N6O6	explosives
178	Selenium	7782-49-2	Se	metals/inorganics
179	Silver	7440-22-4	Ag	metals/inorganics
180	Styrene (Vinyl benzene)	100-42-5	C8H8	hydrocarbons
181	Sulfur Dioxide (SO2)	7446-09-5	O2S	gases
182	Sulfuric Acid	7664-93-9	H2O4S	other
183	Tetrachloroethene	127-18-4	C2Cl4	halogenated
184	Tetryl (2,4,6-trinitrophenylmethylnitramine)	479-45-8	C7H5N5O8	explosives
185	Thallium	7440-28-0	Tl	metals/inorganics
186	Thiophene	110-02-1	C4H4S	hydrocarbons
187	Toluene	108-88-3	C7H8	hydrocarbons
188	trans-2-Butenal	123-73-9	C4H6O	alcohols/ketons
189	trans-2-Butene	624-64-6	C4H8	hydrocarbons
190	trans-2-Pentene	646-04-8	C5H10	hydrocarbons
191	trans-3-Penten-2-one	625-33-2	C5H8O	alcohols/ketones
192	Trichloroethylene (TCE)	79-01-6	C2HCl3	halogenated
193	Trichloroflouromethane	75-69-4	CCl3F	halogenated
194	Vinylidenechloride	75-35-4	C2H2Cl2	halogenated
195	Zinc	7440-66-6	Zn	metals/inorganics

(Sheet 6 of 6)

2 Sources of Physicochemical Data

Several chemical databases are available in the published literature and/or on Internet Web sites. However, some of these databases had insufficient information for the database developed in this project. The data sources selected and used for this project are described in this chapter. Both the physicochemical properties developed here and toxicological benchmark properties developed by CHPPM are included in the database on the CD ROM accompanying this report. The sources of toxicological data are described in Appendix B.

Sources of Data

FRAMES

Framework for Risk Analysis in Multimedia Environmental Systems (FRAMES) (*http://www.pnl.gov/hightechcomm/license/programs/frames.pdf*) (Strenge and Peterson 1989) is software that enables decision-makers and environmental modelers to link their codes with others to perform health impacts and risk assessments. ARAMS uses FRAMES for its system framework. FRAMES is an object-oriented system that contains an *environmental database*. The FRAMES environmental database provides a list of more than 650 contaminants and values for selected physicochemical properties with references. The information from the FRAMES database for the USAEC chemicals is included in the database reported here.

CHPPM

CHPPM (*http://chppm-www.apgea.army.mil/*) has collected physicochemical properties from selected sources for range compounds. These data also were incorporated in the database reported here.

RAIS

Oak Ridge National Laboratory has developed the Risk Assessment Information System (RAIS). RAIS includes a database of selected physicochemical

properties as well as toxicity reference values (*http://risk.lsd.ornl.gov/cgi-bin/tox/TOX_select?select=csf*). These data are included in the database described in this report. The objective of the RAIS database was to provide chemical-specific values needed in the human health risk assessment exposure equations for calculating dose or in the human health risk-based preliminary remediation goal (PRG). RAIS contains information gathered from a variety of sources, which are referenced in the present database. RAIS has the following chemical-specific properties:

a. Gastrointestinal (GI) Absorption Factor (GIAF).

b. Absorption Factor, Dermal (ABS).

c. Diffusivity in Air (D_i).

d. Diffusivity in Water (D_w).

e. Permeability constant (K_p).

f. Soil-Water Partition Coefficient (K_d).

g. Henry's Law Constant (H').

h. Molecular Weight (MW).

i. Organic Carbon Partition Coefficient (K_{oc}).

j. Log of Octanol-water Partition Coefficient (log K_{ow}).

k. Water Solubility (S).

l. Radioactive Half-life (T_R).

m. ICRP Lung Type.

n. GI Absorption Fraction (f_1).

o. Beef Transfer Coefficient (F_b).

p. Fish Bioaccumulation Factor (BF).

q. Milk Transfer Coefficient (F_m).

r. Soil-to-Plant Dry Uptake (Bv_{dry}).

s. Soil-to-Plant Wet Uptake (Bv_{wet}).

PhysProp

The Physical Properties (Physprop) Database (Howard and Meylan 2000) is a database containing physical/chemical properties and chemical structures for more than 22,900 organic chemicals. The following physical/chemical properties are included:

a. Chemical formula.

b. Molecular weight.

c. Melting point/freezing point.

d. Boiling point, water solubility.

e. Log octanol-water partition coefficient.

f. Vapor pressure, dissociation constant (pKa).

g. Henry's law constant.

h. Atmospheric hydroxyl reaction rate constant.

The PhysProp Database is especially useful to scientists in the environmental, pharmaceutical, biochemical, toxicological, and related sciences. These data are included in the present database with reference as the table "PhysProp_Data."

Physical-Chemical Properties Handbook

Another source of data for the database is from *Physical-Chemical Properties and Environmental Fate and Degradation Handbook* (Mackay, Shiu, and Ma 2000). In addition to listing all the many measured and calculated values from the different references, Mackay, Shiu, and Ma (2000) offer suggested values, which are much more useful. The suggested values are based on compilation and review of experimental and estimated data. The suggested property values from the handbook were included in this database.

Mackay, Shiu, and Ma (2000) state, "When compiling the suggested reactivity classes, the authors have examined the available information such as reaction rates of the chemical in each medium by all relevant processes. These were expressed as an overall half-life for transformation. For example, a chemical may be subject to biodegradation with a half-life of 480 hours (rate constant 0.0014 h^{-1}) and photolysis with a half-life of 630 hours (rate constant of 0.0011 h^{-1}). The overall rate constant is thus 0.0025 h^{-1}, and the half-life is 277 hours or 12 days. These half-lives must be used with caution, and it is wise to test the implications of selecting longer and shorter half-lives."

Half-life data in Mackay, Shiu, and Ma (2000) span a range of values for each chemical. However, only the minimum and maximum half-lives were

incorporated in this database. The database displays only the minimum values for the Mackay data source since these values tended to be closer to the values from the other data sources.

Parameter Estimation

Reliable, measured chemical property values are preferred and should be used when available. However, physicochemical property measurements can be difficult, time-consuming, and expensive. Property estimation is becoming a viable alternative to measurements.

Even with the availability of comprehensive experimental data sources, the vast majority of commercial organic chemicals do not have sufficient experimental data to support fate and transport calculations. New or developmental chemicals often have no experimental data available that are relevant to environmental assessments.

Howard (2000) indicated "estimation methods have improved considerably since the early 1980's." As he describes in an editorial note to the Society of Environmental Toxicology and Chemistry 2000 Symposium (Howard 2000), "the user in the past often had to decide which chemical class was the most similar to the chemical being estimated, but the amount of error to be expected for the estimate was unknown. Property estimation methods have become much more sophisticated due to advances in computational tools and our fundamental understanding of the chemical reactions in the environment. The methods now encompass much larger data sets, and users often do not have to select a chemical class."

Howard (2000) also believes that it will be possible for all environmentally relevant properties of all chemicals to be calculated with acceptable accuracy from knowledge only of molecular structure. He indicates that, in general, most physical/chemical/transport/degradation processes that are important to the environmental fate of a chemical can be accurately predicted with a good indication of the error involved (Howard and Meylan 1997). For example, the mean error for several octanol/water partition coefficient estimation methods is close to the experimental error. Processes and properties that have shown good estimated properties include octanol/water partition coefficient, water solubility, vapor pressure, Henry's law constant, the dissociation constant pKa, organic carbon partition coefficient K_{oc}, bioconcentration, and atmospheric oxidation. Methods that still need improvement include biodegradation (only semiquantitative methods are available), photolysis (very limited methods are available), and hydrolysis (methods for limited numbers of chemical classes, such as esters, are available) (Howard and Meylan 1997).

Sources of estimating data

Most current chemical property estimation methods are based upon Quantitative Structure Activity Relationships (QSARs). These methods generally predict the properties of a compound from its chemical structure or other known properties. Computer software can greatly reduce the time and cost necessary to generate properties for acceptable environmental assessment. Table 4 provides references for selected environmental property estimation software. Table 5 shows the properties estimated by various software packages.

Table 4
Environmental Assessment Software

Company	Software	Web Site
EPA	EPI Suite	http://www.epa.gov/oppt/exposure/docs/episuitedl.htm
University of Georgia Dept. of Chemistry	SPARC	http://ibmlc2.chem.uga.edu/sparc/
Advanced Chemistry Development, Inc.	The Physico-Chemical Laboratory	http://www.acdlabs.com/
CambridgeSoft	ChemProp for CS ChemDraw Pro	http://www.camsoft.com
Daylight Chemical Information Systems, Inc., & BloByte Corp.	ClogP	http://www.daylight.com or http://www.biobyte.com/
Interactive Analysis	LogP/LogW	http://www.interactiveanalysis.com

Table 5
Properties Estimated by Various Software Packages

Software	MP	BP	VP	K_{ow}	W_{sol}	HLC	K_{oc}	BCF	OH	Bio	pKa
EPI Suite	X	X	X	X	X	X	X	X	X	X	-
SPARC	-	X	X	X	-	X	-	-	-	-	X
Physico-Chemical Laboratory	-	-	X	X	X	-	-	-	-	-	X
ChemProp for CS ChemDraw	X	X	-	X	-	X	-	-	-	-	-
ClogP	-	-	-	X	-	-	-	-	-	-	-
LogP/LogW	-	-	-	X	X	-	-	-	-	-	-

MP = Melting point; BP = Boiling point; VP = Vapor pressure; K_{ow} = octanol-water partition coefficient; W_{sol} = water solubility; HLC = Henry's Law constant; K_{oc} = organic carbon partition coefficient; BCF = bio-concentration factor (fish); OH = atmospheric oxidation rate; Bio = Biodegradation probability; pKa = dissociation constant.

The handbooks of chemical property estimation methods by Lyman, Reehl, and Rosenblatt (1990) and Boethling and Mackay (1999) include 26 chapters that describe the importance and methods of estimating a variety of physical/chemical properties and transport and degradation processes.

ASTER (*http://www.epa.gov/med/databases/aster.html*) incorporates mechanistically based predictive models to estimate physicochemical properties when these properties are not available through associated databases. The estimates are generated using a QSAR system. The ASTER was developed by the USEPA Mid-Continent Ecology Division to assist regulators with ecological risk assessment.

The Estimation Programs Interface (EPI) is public domain estimation software available to download from a USEPA Web site free of charge (http://www.epa.gov/oppt/exposure/docs/episuitedl.htm). EPI Suite™ (Table 5) includes also the simple environmental models involving sewage treatment plants, Level III fugacity modeling, and volatilization rates from rivers and lakes. A comparison between estimated parameters by EPI and experimental data for selected explosives is given in Chapter 5.

Advantages and disadvantages of QSARS

As indicated previously, the reliable and confirmed measured (experimental) data are preferred if they are available. However, with several thousand chemicals in everyday use and thousands of new synthetic chemicals being developed each year, it is essential to have a method such as QSARs to quickly estimate physicochemical properties. By improving QSAR methods with capability of good error estimation of the prediction, risk assessment and fate and transport calculations could become much less expensive and less resource- and time-consuming. A major drawback of QSAR is that it may rely too much on mathematical formulations, not on experimental results. The property coefficients used in QSARs may be appropriate only for specific types of chemicals, but not for other types of chemicals, which may cause significant errors in estimations. More research and testing are required to develop appropriate formulations that can be applied to a large group of chemicals. Hence, estimated values should be used cautiously.

3 Database Structure

A database was developed using Microsoft Access 2000, included on the accompanying CD. Microsoft Access was chosen because of its availability and versatility as a relational database application and because of time considerations. The majority of the data sources had been prepared using Microsoft Access. The data sources from FRAMES, CHPPM, RAIS, PhysProp, and Mackay, Shiu, and Ma (2000) (see Chapter 2 for details) were incorporated in the database.

Each of the individual data sources was placed into a separate table in the database. A general plan for the comparison of physicochemical properties (such as octanol-water partition coefficient K_{ow} and water solubility) among different data sources was formulated. In addition, the data source structures were modified to show missing values and other information such as temperatures and data types. The missing properties were indicated as not available (N/A).

Information on the specific structure of the data sources that were used in the database can be found in Tables 6-11. These tables indicate the layout of the individual data sources in the database and include some notes on specific areas where data were lacking.

The database includes several tables of the data. Tables 6-11 provide information on type of data included. Table 11 was designed to facilitate the development of the database-user interface that would help future enhancements and/or physicochemical property comparisons with minimal modifications. In general, this table directs the database-user interface on how to gather the appropriate data from the corresponding fields in each data source and how to display the comparison to the user. This table also allows any necessary conversion factors to be applied to provide consistent units among disparate data sources, which may use different units for a given property.

CHPPM provided a data table and associated query for the toxicological data. The toxicological data, which include items such as cancer slope factors and reference doses, were added to the database and used to populate the toxicological data form. Additional details of the CHPPM toxicological data and the structure of this database table may be found in Appendix B.

The database on the CD-ROM displays references for the properties. Some abbreviations in the reference section of CHPPM data are defined here.

a. HS = Hazardous Substances Database.

b. ATS = ATSDR (Agency for Toxic Substances and Disease Registry), *http://www.atsdr.cdc.gov/atsdrhome.html*

c. HZ = Hazard text.

d. CHRIS = Chemical Hazard Response Information System, *http://www.chrismanual.com/*. CHRIS is produced by the U.S. Coast Guard and is available on the *CHEMpendium(TM)* CD-ROM, *http://www.ccohs.ca/products/databases/chris.html*

e. NJ = New Jersey Fact Sheet.

f. RTECS = Registry of Toxic Effects of Chemical Substances (RTECS), *http://www.cdc.gov/niosh/rtecs.html*

Abbreviations for RAIS data reference section of the database are defined as follows:

a. SSL Table C = the USEPA Soil Screening Level Table, *http://risk.lsd.ornl.gov/calc_start.htm*

b. WATER8 has been replaced by WATER9, *http://www.epa.gov/ttn/chief/software/water/index.html*

c. Allen, C.C. (1998) is missing.

d. ASTER: ASTER comes from the MEPAS document.

e. Meylan & Howard, 1993:
Meylan, W.M., and Howard, P.H., *Chemosphere* 26: 2293-99 (1993).

f. Smiley (1981) is missing.

g. Worthing & Walker (1987) is missing.

h. GW CHEM DESK REF, P.16, Montgomery and Welkom, "Groundwater Chemicals Desk Reference," Volumes I and II, 1990.

i. Meylan & Howard (1995). The KowWin Program methodology is described in the following journal article: Meylan, W.M., and P.H. Howard, 1995, "Atom/fragment contribution method for estimating octanol-water partition coefficients," *J. Pharm. Sci.* 84: 83-92.

j. CHEM9: *http://www.epa.gov/ttn/chief/software/chem9/index.html*

k. The "Dermal Prin. and Apps." is "Dermal Exposure Assessment: Principles and Application," Interim Report. EPA/600/8-91/011B, Office of Research and Development, Washington, DC (1992). Link here from *http://risk.lsd.ornl.gov/homepage/epa_hh.shtml*

Table 6
FRAMES Data Fields in the Database

Field Name	Data Type	Description (units)
CAS ID	Text	CAS ID of Chemical
3	Text	RAAS Contaminant Type (N/A)
5	Number	Molecular Weight (g/mole)
6	Text	Melting Point (deg C)
8	Number	Water Solubility (mg/L)
10	Text	Vapor Pressure (mm Hg)
12	Number	Henry's Law Constant (atm m^3/mole)
14	Number	Organic-carbon Partition Coefficient (K_{oc}) (mL/g)
15	Text	Octanol-Water Partition Coefficient (K_{ow}) (mL/mL)
30	Text	Vapor Pressure Temperature (deg C)
31	Text	Diffusion Coefficient in Air (cm^2/s)
32	Text	Diffusion Coefficient in Water (cm^2/s)
37	Text	Inhalation Cancer Potency Factor $(mg/kg/d)^{-1}$
38	Text	Ingestion Cancer Potency Factor $(mg/kg/d)^{-1}$
39	Text	Inhalation Reference Dose (mg/kg/d)
40	Text	Ingestion Reference Dose (mg/kg/d)
41	Text	GI Absorption Fraction (fraction)
42	Text	Inhalation Unit Risk Factor ($risk/ug/m^3$)
43	Text	Inhalation Reference Concentration (mg/m^3)
44	Text	Inhalation Dose Factor, class D (rem/pCi)
48	Text	Ingestion Dose Factor, insoluble (rem/pCi)
49	Text	Dermal Absorption Dose Factor (rem/pCi)
50	Text	External Dose Factor, Air Immersion (rem/hr per pCi/m^3)
51	Text	External Dose Factor, Water Immersion (rem/hr per pCi/L)
52	Text	External Dose Factor, Ground Surface (rem/hr per pCi/m^2)
53	Text	External Dose Factor, Ground Contaminated to 1 cm (rem/hr per pCi/m^3)
56	Text	Inhalation Slope Factor (risk/pCi)
57	Text	Ingestion Slope Factor (risk/pCi)
58	Text	External Exposure Slope Factor (risk/yr per pCi/g soil)
59	Text	Dermal Absorption Fraction from Soil (fraction)
60	Text	Aqueous Skin Permeability (cm/hr)
62	Text	Water Purification Factor (N/A)
63	Text	Deposition Velocity (m/s)
64	Text	Bioaccumulation in Freshwater Fish (L/kg)
66	Text	Bioaccumulation in Freshwater Crustacea (pCi/kg food per pCi/L water)

(Continued)

Table 6 (Concluded)

Field Name	Data Type	Description (units)
72	Text	Feed to Animal Meat Transfer Factor (pCi/kg food per pCi/d intake)
73	Text	Feed to Animal Milk Transfer Factor (pCi/L food per pCi/d intake)
76	Text	Feed to Egg Transfer Factor (pCi/kg food per pCi/d intake)
77	Text	Soil to Plant Concentration Ratio for Root Vegetable (pCi/kg dry plant per pCi/kg soil)
78	Text	Soil to Plant Concentration Ratio for Fruit (pCi/kg dry plant per pCi/kg soil)
79	Text	Soil to Plant Concentration Ratio for Cereal (pCi/kg dry plant per pCi/kg soil)
80	Text	Soil to Plant Concentration Ratio for Animal Forage (pCi/kg dry plant per pCi/kg soil)
81	Text	Soil to Plant Concentration Ratio for Hay (pCi/kg dry plant per pCi/kg soil)
82	Text	Soil to Plant Concentration Ratio for Grain (pCi/kg dry plant per pCi/kg soil
83	Text	Half Time in Air (days)
84	Text	Half Time in Groundwater (days)
85	Text	Half Time in Surface Water (days)
86	Text	Half Time in Soil (days)
97	Text	Atmospheric Deposition Class (N/A)
98	Text	MEPAS Contaminant Type (N/A)
99	Text	Contaminant Name (N/A)
100	Text	GI Absorption Fraction, Insoluble (N/A)
101	Text	Soil to Plant Concentration Ratio, Other Vegetables (pCi/kg dry plant per pCi/kg soil)
105	Text	Pure Contaminant Density (g/mL)
110	Text	Contaminant Type (n/a)
138	Text	Ingestion Unit Risk Factor (risk/ug/L)
139	Text	Grout Diffusion Coefficient (cm^2/s)

Table 7
CHPPM Data Fields in the Database

Field Name	Data Type	Description
Chemical	Text	Substance
CAS #	Text	CAS Number
CAS ID	Text	CAS ID = CAS NUMBER without -
Molecular Weight	Text	Molecular Weight
Ref-Mol	Text	Reference for Molecular Weight
Chem- State	Text	Chemical State (Solid, liquid, gas)
Ref-State	Text	Reference for Chemical State
Henry's Law	Text	Henry's Law Constant (atm m3 /mole)
Temp-Henry's Law	Text	Temperature for Henry's Law Constant (°C)
Ref-Henry	Text	Reference for Henry's Law
Water Solub (mg/L)	Text	Water Solubility (mg/l)
Tem-Water Solu	Text	Temperature for Water Solubility (°C)
Ref-Water Solu	Text	Reference for Water Solubility
Vapor Pressure (mm Hg or torr)	Text	Vapor Pressure (mm Hg or torr @ temp)
Temp-Vapor Pressure	Text	Temperature of Vapor Pressure
Ref-Vapor Pressure	Text	Reference for Vapor Pressure
Oct/Water (log K_{ow})	Text	Oct/Water coefficient (unitless)
Ref-K_{ow}	Text	Reference for K_{ow}
K_{oc} (L/kg)	Text	K_{oc} (C part. Coefficient)
K_{oc}-Calculation way	Text	K_{oc} data type (measured or estimated)
Ref-K_{oc}_CHPPM	Text	Reference for K_{oc}
ABC	Text	Absorption factor, dermal (unitless)
Aqueous Skin Permeability	Text	Aqueous Skin Permeability (cm/hr)
GI Abs Fraction	Text	GI Absorption Fraction, f1 (unitless)
Soil ½ Life (days)	Text	Half-Life in Soil (days)
Est Soil 1/2 Life (days)	Text	Estimated Half-Life in Soil (days)
GW ½ life (days)	Text	Half-Life in Groundwater (days)
Ing RfDo	Text	Oral Reference Dose (mg/kg/d)
Ref-Ing RfDo	Text	Reference for Oral Reference Dose
CSFo	Text	Cancer Slope Factor (1/mg/kg/d)
Ref-CSFo	Text	Reference for Cancer Slope Factor
Inh RfDi	Text	Inhalation Reference Dose (mg/kg/d)
Ref-Inh RfDi	Text	Reference for Inhalation Reference Dose
CSFi	Text	Cancer Slope Factor Inhalation (1/mg/kg/d)
Ref-CSFi	Text	Reference for Cancer Slope Factor Inhalation
TWA	Text	The Allowable Time-Weighted Average Concentration

Table 8
RAIS Data Fields in the Database

Field Name	Data Type	Description
ID	AutoNumber	Chemical ID
Chemical	Text	Chemical Name
CAS ID	Text	CAS Number
Absorption Factor, Dermal	Number	Absorption Factor, Dermal
Ref_ABFD	Text	Reference for Absorption Factor, Dermal
Beef Transfer Coeff (day/kg)	Number	Beef Transfer Coefficient (day/kg)
Ref_BTC	Text	Reference for Beef Transfer Coefficient (day/kg)
Soil-to-Dry Plant Uptake	Number	Soil to Dry Plant Uptake
Ref_SDPU	Text	Reference for Soil to Dry Plant Uptake
Soil-to-Wet Plant Uptake	Number	Soil to Wet Plant Uptake
Ref_SWPU	Text	Reference for Soil to Wet Plant Uptake
Diffusivity in Air (cm2/s)	Number	Diffusivity in Air (cm2/s)
Ref_DA	Text	Reference for Diffusivity in Air (cm2/s)
Diffusivity in Water (Cm2/s)	Number	Diffusivity in Water (Cm2/s)
Ref_DW	Text	Reference for Diffusivity in Water (Cm2/s)
Fish Bioacc Factor (L/kg)	Number	Fish Bioacc Factor (L/kg)
Ref_FBF	Text	Reference for Fish Bioacc Factor (L/kg)
GI Absorption Factor	Number	GI Absorption Factor
Ref_GIAF	Text	Reference for GI Absorption Factor
GI Absorption Fraction (f1)	Text	GI Absorption Fraction (f1)
Ref_GIAFf1	Text	GI Absorption Fraction (f1), Reference
Radioactive half-life (days)	Number	Radioactive half-life (days)
Ref_Rhlife	Text	Radioactive half-life (days), Reference
Unitless Henry's Law Constant	Number	Unitless Henry's Law Constant
Ref_HLC	Text	Unitless Henry's Law Constant, Reference
Soil-Water Partition Coef (cm3/g)	Text	Soil-Water Partition Coef (cm3/g)
Ref_SWP	Text	Soil-Water Partition Coef (cm3/g), Reference
Organic Carbon Partition Coef (L/kg)	Number	Organic Carbon Partition Coef (L/kg)
Ref_Koc_Oak	Text	Organic Carbon Partition Coef (L/kg), Reference
Permeability Constant (cm/hr)	Number	Permeability Constant (cm/hr)
Ref_PC	Text	Permeability Constant (cm/hr), Reference
Log of Octanol-Water Partition Coef	Number	Log of Octanol-Water Partition Coefficient
Ref_Lkow	Text	Log of Octanol-Water Partition Coefficient, Reference
ICRP Lung Type F	Text	ICRP Lung Type F
Ref_ICRP	Text	ICRP Lung Type F, Reference
Milk Transfer Coeff (day/kg)	Number	Milk Transfer Coeff (day/kg)
Ref_MTC	Text	Milk Transfer Coeff (day/kg), Reference
Molecular Weight	Number	Molecular Weight
Ref_MW	Text	Molecular Weight, Reference
Water Solubility (mg/L)	Number	Water Solubility (mg/L)
Ref_WS	Text	Water Solubility (mg/L), Reference
DefaultValue	Text	Default Value
DefaultReference	Text	Default Reference
DefaultTemp	Text	Default Temperature, deg C
DefaultEstimate	Text	Default Estimate Indicator

Table 9
PhysProp Data Fields in the Database

Field Name	Data Type	Description (unit)
CAS #	Text	CAS Number with - between numbers
Formula	Text	Chemical Formula
Mol Weight	Number	Molecular Weight
Chemical Name	Text	Chemical Name
WS (mg/L)	Number	Water Solubility (mg/L)
WS_temp	Number	Water Solubility Temperature (deg C)
WS_type	Text	Water Solubility Type (EXP = experimentally measured or derived data; EST = estimated data; EXT = extrapolated data)
WS_reference	Text	Water Solubility Reference
LogP	Number	log K_{ow} (Log Octanol-Water Partition Coefficient (log P))
LogP_temp	Number	log K_{ow} Temperature (deg C)
LogP_type	Text	log K_{ow} Type
LogP_reference	Text	log K_{ow} Reference
VP (mm Hg)	Number	Vapor Pressure (mm Hg)
VP_temp	Number	Vapor Pressure Temperature
VP_type	Text	Vapor Pressure Type
VP_reference	Text	Vapor Pressure Reference
DC_pKa	Number	Dissociation Constant
DC_temp	Number	Dissociation Constant Temperature (deg C)
DC_type	Text	Dissociation Constant Data Type
DC_reference	Text	Dissociation Constant Reference
HL (atm-m3/mole)	Number	Henry's Law Constant (atm m^3/mole)
HL_temp	Number	Henry's Law Constant Temperature (deg C)
HL_type	Text	Henry's Law Constant Type
HL_reference	Text	Henry's Law Reference
OH (cm3/molecule-sec)	Number	Atmospheric Hydroxyl Radical Reaction Rate Constant (cm^3/molecule-sec)
OH_temp	Number	Atmospheric Hydroxyl Radical Reaction Rate Constant Temperature
OH_type	Text	Atmospheric Hydroxyl Radical Reaction Rate Constant Data Type
OH_reference	Text	Atmospheric Hydroxyl Radical Reaction Rate Constant Reference
BP_pressure (mm Hg)	Number	Boiling Point Pressure (mm Hg)
MP (deg C)	Text	Melting Point (deg C)
BP (deg C)	Number	Boiling Point (deg C)
FP (deg C)	Text	Freezing Point (deg C)
DefaultValue	Text	Default Value
DefaultReference	Text	Default Reference
DefaultTemp	Text	Default Temperature, deg C
DefaultEstimate	Text	Default Estimate Indicator

Table 10
Mackay, Shiu, and Ma (2000) Book_Data Fields in the Database

Field Name	Data Type	Description
ID	AutoNumber	ID Number
Chemical_Book	Text	Chemical Name
CAS #	Text	CAS Numbers
log Kow	Text	Log of Octanol-Water Partition Coefficient
Solubility (g/m3)	Text	Solubility in Water (g/m^3)
Vapor Pressure (Pa)	Text	Vapor Pressure in Pa
Henry's Constant (Pa m3/mol)	Text	Henry's Law Constant in Pa m^3/mol
Half_Air (class)	Text	Class of Half-life in Air
Half_Water (class)	Text	Class of Half-life in Water
Half_Soil (class)	Text	Class of Half-life in Soil
Half_Sediment (class)	Text	Class of Half-life in Sediment
Default Value	Text	Default Value
Default Reference	Text	Default Reference
Default Temp	Text	Default Temperature, deg C
Default Estimate	Text	Default Estimate Indicator
Table used for classes related to half-life times		
ID	Auto Number	ID Number
Class	Text	Class or Range of Parameter Values
half_min (hours)	Text	Minimum Half-Life for Given Parameter
half_max (hours)	Text	Maximum Half-Life for Given Parameter

Note: Units are consistent with other data source tables and Appendix C.

Table 11
Table for User Interface and Interrelationship of Data Sources

Field Name	Data Type	Description
ID	AutoNumber	Unique ID
QueryName	Text	The name of query
NumTables	Number	The number of data sources to perform query upon
DataSource1Title	Text	Title to show for Data Source # 1
DataSource2Title	Text	Title to show for Data Source #2
DataSource3Title	Text	Title to show for Data Source #3
DataSource4Title	Text	Title to show for Data Source #4
DataSource5Title	Text	Title to show for Data Source #5
Table1Name	Text	The name of first Table to be used in query
Tbl1VarColName	Text	The name of the column of the variable to be used in query
Tbl1VarDataType	Text	Variable data type
Tbl1PrefixRequired	Yes/No	Is conversion prefix required?
Tbl1Prefix	Text	Prefix to use (e.g. log())
Tbl1ConvRequired	Yes/No	Is conversion factor required?
Tbl1ConvFactor	Number	Conversion factor
Tbl1EstColName	Text	Name of column to use for whether the variable is estimated, extrapolated, etc.
Table2Name	Text	The name of second Table to be used in query
Tbl2VarColName	Text	The name of the column of the variable to be used in query
Tbl2VarDataType	Text	Variable data type
Tbl2PrefixRequired	Yes/No	Is conversion prefix required?
Tbl2Prefix	Text	Prefix to use (e.g. log())
Tbl2ConvRequired	Yes/No	Is conversion factor required?
Tbl2ConvFactor	Number	Conversion factor
Tbl2EstColName	Text	Name of column to use for whether the variable is estimated, extrapolated, etc.

4 Database-User Interface

A user interface was designed using Microsoft Access to present data in a user-friendly manner that can be viewed, but not edited. This interface integrates the tables of data in the database and provides easy access to the data. The use of this database requires Microsoft Access software installed on the user's computer. When the user first loads the application, a dialog is displayed that allows the user to access either physicochemical data or toxicological data (Figure 1). This main dialog also contains features for **Page Setup** and **Print Preview**, as well as **Compact and Repair Database**, which are accessible from the **File** and **Utilities** menus, respectively. Selecting **Physicochemical Data** brings up a dialog box like that shown in Figure 2. Selecting **Toxicological Data** brings up a dialog box like that shown in Figure 3.

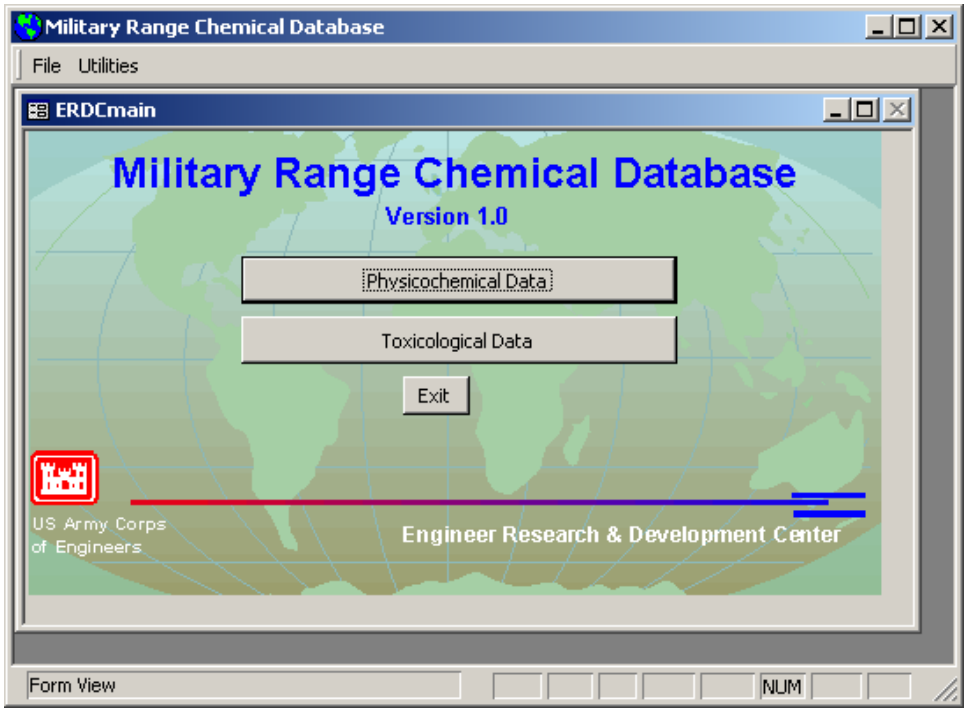


Figure 1. The main dialog

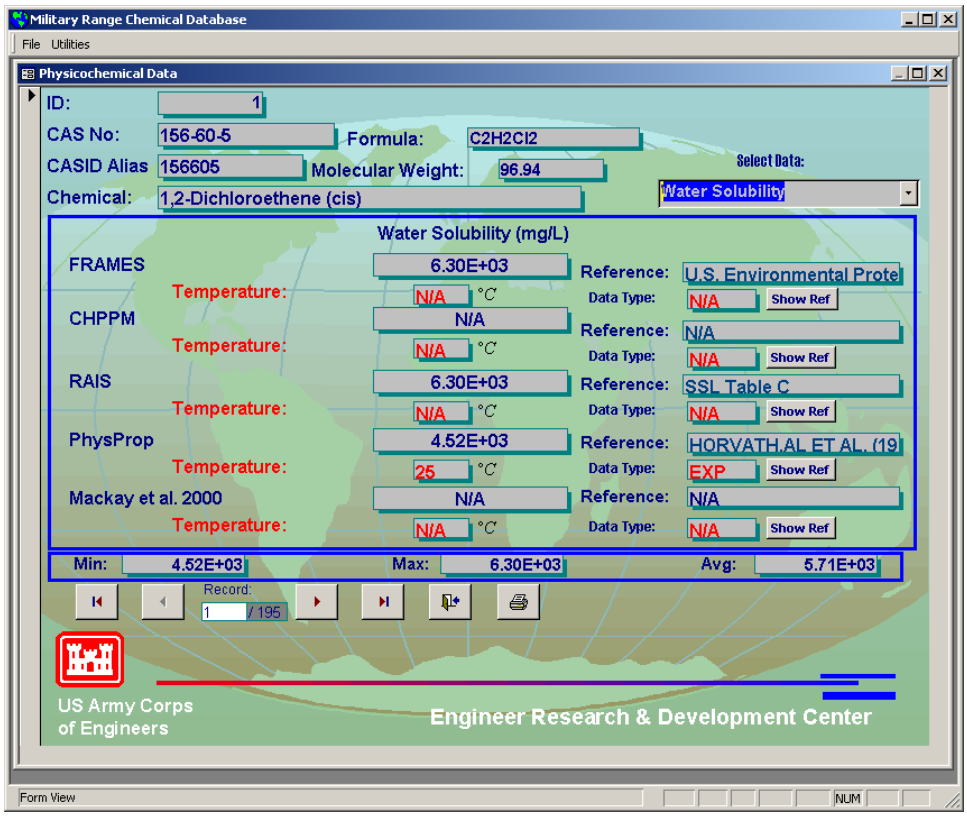


Figure 2. The **Physicochemical Data** dialog screen

The **Physicochemical Data** form displays a wealth of information integrated from the multiple data sources described in Chapter 2. The basic idea for the operation of this form is to navigate to a particular chemical of interest using the record navigation buttons located on the bottom left side of the form as shown in Figure 4. Once the chemical of interest has been chosen, the user can choose the property of interest by selecting from the list of values displayed in the **Select Data** drop-down menu. Currently eleven properties are available: aqueous skin permeability, K_{ow}, K_{oc}, GI absorption fraction-insoluble, half-life in air, half-life in groundwater, half-life in soil, half-life in surface water, Henry's law constant, vapor pressure, and water solubility. Once the property of interest has been chosen, the form will update itself with the values from the various sources in the database. The database on the screen also indicates the temperatures associated with the property, if appropriate and available, as well as short references from each data source. In addition, the database provides the data type (estimated (EST), extrapolated (EXT), not available (N/A), measured or experimental (EXP)) and a **Show Ref** button, which display the complete (detail) reference for the property. The form also displays the average, minimum, and maximum values obtained from the various data sources for the selected property. The user can exit (Figure 5) or print the form (Figure 6) by pressing the appropriate button.

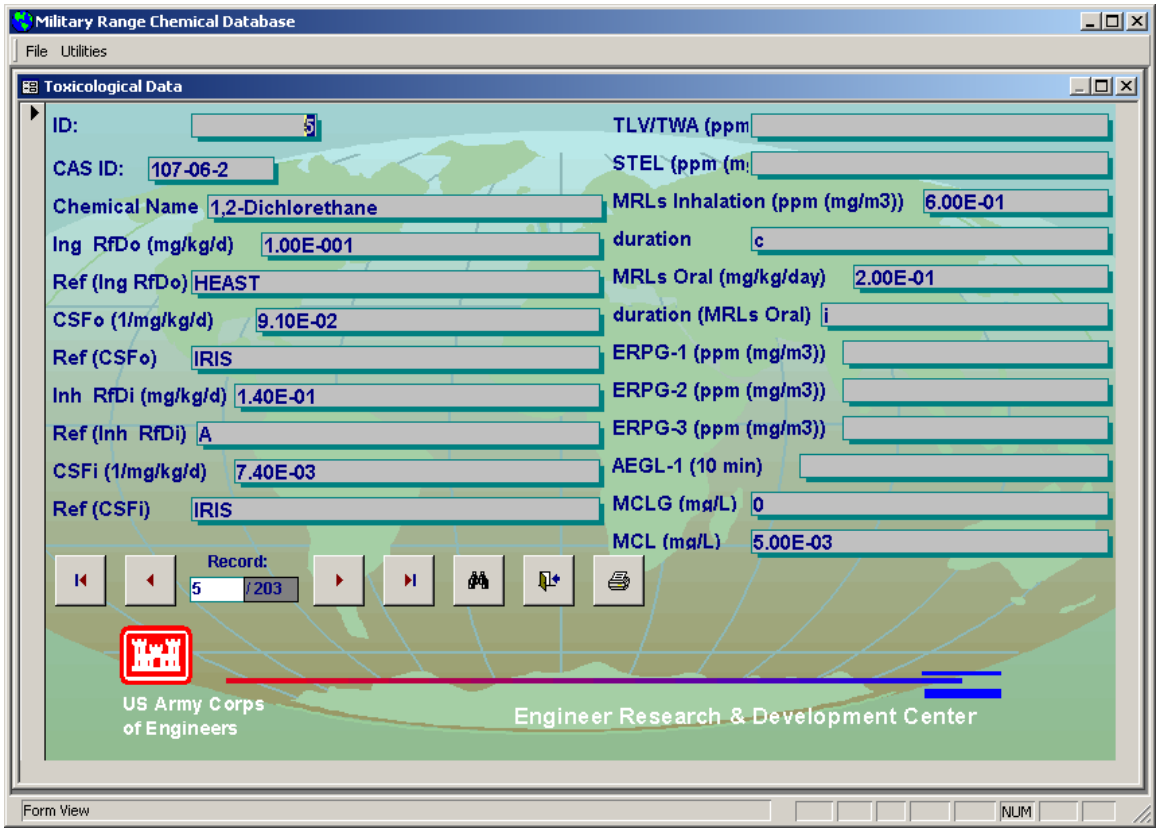


Figure 3. The **Toxicological Data** dialog screen

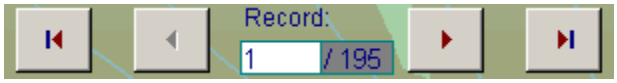


Figure 4. The form record navigation buttons

Figure 5. The form **Exit** button

Figure 6. The form **Print** button

The **Toxicological Data** option accesses various toxicological data. Navigation of this form to a particular chemical is similar to that of **Physicochemical Data**, and the screen also contains buttons to exit and print the form. This form is structured differently from the previous in that all the toxicity values for a particular chemical are presented on a single page without the need for a combo box to select a particular toxicological property. The data used for this form include the following:

a. Ingestion reference dose (Ing. RFDo).

b. Inhalation reference dose (Inh. RFDi).

c. Threshold Limit Value/Time Weighted Average (TWA).

d. Short-Term Exposure Levels (STEL).

e. Ingestion Minimal Risk Levels and Duration (MRLs Oral).

f. Inhalation Minimal Risk Levels and Duration (MRLs Inhalation).

g. Emergency Response Planning Guidelines (ERPG-1, ERPG-2, ERPG-3).

h. Levels 1-3, Acute Exposure Guideline Level 1 (AEGL-1).

i. Maximum Contaminant Levels (MCL).

j. Maximum Contaminant Level Goals (MCGLs).

k. Oral Cancer Slope Factor (CSFo).

l. Inhalation Cancer Slope Factor (CSFi).

The toxicological benchmark data in the database were provided by CHPPM. The report for the toxicological data is provided in Appendix B.

5 Results and Analysis

The data collected under this project are provided in a Microsoft Access 2000 file on the accompanying CD ROM. A statistical analysis that calculates and displays the range of data (minimum, average, maximum) is also included in the database. This chapter includes a section on the availability of property values and a section on comparison of measured and estimated values for a few representative properties and chemicals.

Availability of Property Values

Initially, 28 parameters were selected for the data compilation (Table 12). However, many of these parameters were not available, although some of them could be calculated using available estimation software and formulations. Currently, only the first 11 chemical properties (parameters 3-13 in Table 12) are included in the database. The database is very flexible and additional data can be added to the database in the future. The included parameters are classified as transport, exposure, and decay parameters (Table 12).

In addition to the five main sources of data as described in Chapter 2, another set of data on half-lives is provided in Appendix A. Explosives data are provided in Brannon and Pennington (2002) and Miyares and Jenkins (2000). Solubility and K_{ow} data from Brannon and Pennington (2002) were used in a comparison with estimated values as discussed in the next section. In general, the half-life data and particularly half-life in groundwater and toxicity data have significant gaps.

The five sources of data that were incorporated into the database (Chapter 2) were checked for availability (existence) of property values for the 11 physicochemical parameters octanol-water partition coefficient K_{ow}, water solubility, vapor pressure, Henry's law constant, aqueous skin permeability, GI absorption fraction (insoluble), half-life in air, half-life in groundwater, half-life in soil, half-life in surface water, and carbon matter partition coefficient K_{oc}. The results of the properties search are given in Table 13.

Table 13 lists chemicals with Chemical Abstract Service (CAS) number and number of data values for each selected physicochemical property. The last column in Table 13 provides information on the number of properties among the 11 that currently have data in the database. For example the number 11 means that all 11 selected parameters have at least one value in the database. A number

Table 12
Parameter Ranking of Selected Physicochemical Parameters Being Addressed in This Study

Parameter	Ranking	Property
Parameter Ranking (highest priority)		
Transport	1	Contaminant Type
	2	Molecular Weight
	3	Octanol-Water Partition Coefficient (K_{ow})
	4	Water Solubility
	5	Vapor Pressure
	6	Henry's Law Constant
Exposure	7	Aqueous Skin Permeability
	8	GI Absorption Fraction
Decay	9	Half-Life in Air
	10	Half-Life in Groundwater
	11	Half-Life in Soil
	12	Half-Life in Surface Water
Transport	13	Organic Carbon Partition Coefficient (K_{oc})
	14	Dissolution Rate[1]
Parameter Ranking (lower priority)		
Transport	15	Atmospheric Deposition Class
	16	Deposition Velocity
Transfer to food	17	Bioaccumulation in Freshwater Crustacea
	18	Bioaccumulation in Freshwater Fish
	19	Feed to Animal Meat Transfer Factor
	20	Feed to Animal Milk Transfer Factor
	21	Soil to Plant Concentration Ratio for Animal Forage
	22	Soil to Plant Concentration Ratio for Cereal
	23	Soil to Plant Concentration Ratio for Fruit
	24	Soil to Plant Concentration Ratio for Grain
	25	Soil to Plant Concentration for Hay
	26	Soil to Plant Concentration Ratio for Leafy Vegetables
	27	Soil to Plant Concentration Ratio for Root Vegetables
	28	Soil to Plant Concentration Ratio, Other Vegetables

[1] This information is not included in the current version of the database

0 means no values were available for the property. Table 14 summarizes the information of Table 13 and shows the percentage of chemicals versus parameters available in the database. The most sparsely populated portions of the database are from the half-lives and particularly the half-life in groundwater and toxicity data.

Table 13
Number of Values Found for Each Property and Number of Properties Included in the Database, in Decreasing Order of Completeness

ID	Chemicals-USAEC	CAS ID	K_{ow}	W_{sol}	VP	HLC	ASP	GI	HA	HG	HS	HSW	K_{oc}	Number of Available Parameters
7	1,2-Dichloroethene (cis/trans MIXTURE)	540-59-0	3	2	2	2	1	1	2	1	1	1	1	11
25	2,3,7,8-Tetrachlorodibenzo-p-Dioxin	1746-01-6	5	5	4	5	3	2	2	1	1	3	3	11
40	2-Propanol	67-63-0	5	2	4	5	3	2	1	1	3	3	3	11
51	4-Methyl-2-Pentanone	108-10-1	4	5	4	5	3	2	2	1	2	3	3	11
59	Acetonitrile	75-05-8	5	3	4	5	3	2	3	1	2	3	3	11
60	Acetophenone	98-86-2	5	5	4	5	3	2	2	2	2	3	3	11
62	Acrolein	107-02-8	5	5	4	5	3	2	2	1	4	3	2	11
63	Acrylonitrile	107-13-1	4	4	4	5	3	2	3	1	2	3	3	11
71	Benzene	71-43-2	5	5	4	5	3	2	2	1	3	2	3	11
81	Bis(2-ethylhexyl)phthalate	117-81-7	5	5	4	5	3	2	2	1	2	2	3	11
88	Carbon tetrachloride	56-23-5	5	5	4	5	3	2	3	2	3	3	3	11
91	Chloroethene (Vinyl chloride)	75-01-4	5	5	4	5	3	2	2	1	3	2	3	11
106	Dioctyl phthalate	117-81-7	5	5	4	5	3	2	2	1	2	2	3	11
107	Dioxin TEQ (c)	1746-01-6	5	5	4	5	3	2	2	1	2	3	3	11
110	Ethanol	64-17-5	4	2	4	4	2	1	3	1	2	3	2	11
111	Ethylbenzene	100-41-4	5	5	4	5	3	2	2	1	3	2	3	11
112	Ethylchloride	75-00-3	5	5	4	5	3	2	2	2	3	3	3	11
121	Hexachlorobutadiene	87-68-3	4	4	3	4	3	2	1	1	1	1	3	11
123	Hexachloroethane	67-72-1	5	5	4	5	3	2	2	1	2	3	3	11
135	p-Xylene (para-xylene)	106-42-3	4	3	3	4	3	2	1	1	2	1	3	11
144	Methyl-t-butylether (MTBE)	1634-04-4	4	4	3	4	2	1	2	1	1	1	2	11
146	Naphthalene	91-20-3	5	5	4	5	3	2	2	2	3	3	3	11
160	o-Dichlorobenzene	95-50-1	5	5	4	5	3	2	2	1	2	2	3	11
180	Styrene (Vinyl benzene)	100-42-5	5	5	4	5	3	2	3	1	3	2	3	11
187	Toluene	108-88-3	5	4	4	5	3	2	2	1	4	3	3	11
193	Trichloroflouromethane	75-69-4	5	5	4	5	3	2	2	1	4	2	3	11
4	1,2,4-Trimethylbenzene	95-63-6	4	4	3	4	2	1	2	0	1	2	2	10
5	1,2-Dichlorethane	107-06-2	5	5	4	5	3	2	3	0	2	2	3	10
8	1,3,5-Trimethylbenzene (MESITYLENE)	108-67-8	4	4	3	4	2	1	2	0	1	1	2	10
10	1,3-Butadiene	106-99-0	5	5	4	5	3	2	2	0	1	2	3	10
11	1,3-Dinitrobenzene	99-65-0	4	4	3	4	2	2	1	0	1	2	2	10
14	1-Butanol	71-36-3	5	5	4	5	3	2	2	0	2	2	3	10
26	2,4,6-Trinitrotoluene (TNT)	118-96-7	3	4	3	3	2	2	1	0	1	2	2	10
27	2,4-Dinitrotoluene (DNT; 2,4-DNT)	121-14-2	4	4	3	4	2	2	1	0	2	3	2	10
32	2-Butanone	78-93-3	5	5	4	5	3	2	2	0	2	3	3	10
33	2-Furaldehyde	98-01-1	4	4	3	4	2	1	1	0	1	1	2	10
38	2-Nitrotoluene (ONT)	88-72-2	4	3	3	4	2	2	2	0	1	3	2	10
52	4-Nitrotoluene	99-99-0	3	3	2	3	1	1	1	0	1	1	1	10

(Sheet 1 of 5)

Note: K_{ow} - Octanol-water partitioning coefficient; W_{sol} - Solubility; VP - Vapor Pressure; HLC - Henry's law constant; ASP - Aqueous_Skin_Permeability;
GI - GI_Absorption_Insoluble; HA - Half-life_Air; HG - Half-life Groundwater; HS - Half-life_Soil; HSW - Half-life_Surface Water; K_{oc} - Organic carbon partition coefficient.

Table 13 (Continued)

ID	Chemicals-USAEC	CAS ID	K_{ow}	W_{sol}	VP	HLC	ASP	GI	HA	HG	HS	HSW	K_{oc}	Number of Available Parameters
54	Acenaphthene	83-32-9	4	4	3	4	2	2	1	0	1	1	2	10
55	Acenaphthylene	208-96-8	5	5	4	5	3	2	1	0	4	3	3	10
56	Acetaldehyde	75-07-0	3	3	3	4	2	1	2	0	1	2	2	10
57	Acetic Acid	64-19-7	3	2	3	3	1	0	2	1	2	1	1	10
58	Acetone	67-64-1	5	3	4	5	3	2	2	0	2	3	3	10
65	Anthracene	120-12-7	4	4	3	4	2	2	2	0	2	3	2	10
69	Benzaldehyde	100-52-7	5	4	4	5	3	2	2	0	2	1	3	10
72	Benzo(a)anthracene	56-55-3	4	4	3	4	2	2	1	0	2	3	2	10
73	Benzo(a)pyrene	50-32-8	4	4	3	4	2	2	1	0	2	3	2	10
77	Benzo(k)fluoranthene	207-08-9	4	4	3	4	2	2	1	0	2	2	2	10
84	Calcium	7440-70-2	2	1	2	2	1	1	1	0	1	1	1	10
86	Carbon Disulfide	75-15-0	4	5	4	5	3	2	2	0	2	2	3	10
90	Chlorobenzene	108-90-7	5	5	4	5	3	2	3	0	3	2	3	10
92	Chloroform	67-66-3	5	5	4	5	3	2	2	0	2	2	3	10
93	Chloromethane	74-87-3	4	4	3	4	2	2	2	0	2	3	2	10
95	Chrysene	218-01-9	4	4	3	4	2	2	1	0	2	3	2	10
97	Cl2 (a)	7782-50-5	2	2	3	2	2	2	1	0	1	1	1	10
100	Dibenz(a,h)anthracene	53-70-3	4	4	3	3	2	2	1	0	2	2	2	10
102	Dibutyl phthalate	84-74-2	5	5	4	5	3	2	2	0	2	2	3	10
104	Dichlorodiflouromethane	75-71-8	5	5	4	5	3	2	2	0	2	2	3	10
108	Diphenylamine	122-39-4	4	4	3	4	2	2	1	0	2	2	2	10
109	Ethane	74-84-0	3	3	3	3	2	1	1	0	1	1	2	10
114	Fluoranthene	206-44-0	4	4	3	4	2	2	1	0	2	2	2	10
115	Fluorene	86-73-7	5	4	4	5	3	2	2	0	3	3	3	10
116	Formaldehyde	50-00-0	4	3	3	4	2	2	2	0	2	2	2	10
117	Furan	110-00-9	5	5	4	5	3	2	2	0	2	2	3	10
120	Hexachlorobenzene	118-74-1	5	5	4	5	3	2	2	0	3	2	3	10
122	Hexachlorocyclopentadiene	77-47-4	4	4	3	4	3	2	0	1	1	1	3	10
125	Hexane	110-54-3	5	5	4	5	3	2	2	0	2	2	3	10
127	Hydrogen Cyanide	74-90-8	3	3	2	3	2	2	1	0	1	1	1	10
128	i-Butane (isobutane)	75-28-5	3	3	3	3	1	1	2	0	1	1	1	10
134	m-Xylene (meta-xylene)	108-38-3	4	4	3	4	3	2	0	1	1	1	3	10
138	m-Dichlorobenzene	541-73-1	5	5	4	4	3	2	2	0	2	3	3	10
142	Methylene Chloride	75-09-2	5	5	4	5	3	2	2	0	2	2	3	10
147	n-Butane	106-97-8	4	4	4	4	2	1	2	0	1	1	2	10
150	n-Hexane	110-54-3	5	5	4	5	3	2	2	0	2	2	3	10
153	Nitrobenzene	98-95-3	5	5	4	5	3	2	2	0	2	3	3	10
158	OCDD (1,2,3,4,6,7,8,9-OCDD)	3268-87-9	4	3	3	3	2	2	1	0	2	1	2	10
162	o-Xylene (ortho-xylene)	95-47-6	5	5	4	5	3	2	2	0	2	2	3	10
164	p-Dichlorobenzene (para-Dichlorobenzene)	106-46-7	5	5	4	5	3	2	2	0	2	2	3	10
166	Perchloroethylene	127-18-4	5	5	4	5	3	2	2	0	2	2	3	10
167	Phenanthrene	85-01-8	5	5	4	5	3	2	2	0	2	3	3	10

(Sheet 2 of 5)

Table 13 (Continued)

ID	Chemicals-USAEC	CAS ID	K_{ow}	W_{sol}	VP	HLC	ASP	GI	HA	HG	HS	HSW	K_{oc}	Number of Available Parameters
168	Phenol	108-95-2	5	5	4	5	3	2	3	0	2	3	3	10
172	Propane	74-98-6	3	3	3	3	2	1	1	0	1	1	2	10
176	Pyrene	129-00-0	4	4	3	4	2	2	1	0	2	3	2	10
177	RDX	121-82-4	3	3	2	2	2	2	1	0	1	1	2	10
183	Tetrachloroethene	127-18-4	5	5	4	5	3	2	2	0	2	2	3	10
192	Trichloroethylene (TCE)	79-01-6	5	5	4	5	3	2	2	0	2	2	3	10
194	Vinylidenechloride	75-35-4	5	5	4	5	3	2	2	0	2	2	3	10
2	1,2-Dichloroethene (trans)	156-60-5	3	3	2	3	2	2	0	0	1	1	2	9
9	1,3,5-Trinitrobenzene	99-35-4	3	3	2	3	2	2	1	0	0	2	2	9
20	1-Pentene	109-67-1	3	3	3	3	1	0	2	0	1	1	1	9
28	2,6-Dinitrotoluene (2,6-DNT)	606-20-2	3	3	2	3	1	1	1	0	0	1	1	9
34	2-Heptanone	110-43-0	3	3	3	3	1	0	2	0	1	1	1	9
39	2-Pentanone	107-87-9	3	3	3	3	1	0	2	0	1	1	1	9
47	3-Nitrotoluene	99-08-1	3	2	2	3	1	1	1	0	0	1	1	9
64	Aluminum	7429-90-5	1	1	2	1	2	2	1	0	1	0	1	9
66	Antimony	7440-36-0	2	3	3	2	2	2	1	0	1	0	1	9
74	Benzo(b)fluoranthene	205-99-2	4	4	2	3	2	2	0	0	1	1	2	9
82	Butanal	123-72-8	3	3	3	3	1	0	2	0	1	1	1	9
126	HMX	2691-41-0	3	2	2	2	2	2	0	0	1	1	2	9
130	Indeno(1,2,3-cd)pyrene	193-39-5	3	3	2	3	2	2	0	0	1	1	2	9
133	Xylene (mixed isomers)	1330-20-7	3	2	2	3	2	2	0	0	1	1	2	9
148	n-Decane	124-18-5	3	3	3	3	1	0	2	0	1	1	1	9
165	Pentaerythritoltetranitrate (PETN)	78-11-5	2	2	2	2	1	1	0	0	1	1	1	9
171	Propanal	123-38-6	3	3	3	3	1	0	2	0	1	1	1	9
3	(1,2-dichloroethyl) benzene	1074-11-9	2	1	1	1	1	0	1	0	0	1	1	8
16	Isobutylene	115-11-7	3	3	3	3	1	0	2	0	0	1	1	8
30	2-Amino-4,6-Dinitrotoluene	35572-78-2	1	1	1	1	1	2	0	0	0	1	1	8
35	2-Methyl-1-butene	563-46-2	3	3	3	3	1	0	1	0	0	1	1	8
50	4-Ethyltoluene	622-96-8	3	3	3	3	1	0	1	0	0	1	1	8
67	Arsenic	7440-38-2	2	3	3	2	2	2	0	0	1	0	1	8
68	Barium	7440-39-3	2	3	3	1	2	2	0	0	1	0	1	8
75	Benzo(e)pyrene	192-97-2	2	3	3	3	1	1	0	0	1	0	1	8
80	Beryllium	7440-41-7	2	2	3	2	2	2	0	0	1	0	1	8
83	Cadmium	7440-43-9	2	2	3	2	2	2	0	0	1	0	1	8
94	Chromium	7440-47-3	2	1	3	1	1	1	0	0	1	0	1	8
98	Cobalt	7440-48-4	2	2	3	1	2	2	0	0	1	0	1	8
99	Copper	7440-50-8	2	2	3	2	2	2	0	0	1	0	1	8
113	Ethylene	74-85-1	2	2	2	2	1	0	1	1	0	0	1	8
118	HCl	7647-01-0	1	2	2	1	2	2	0	0	1	0	1	8
129	i-Butene (isobutene/E-butylene)	115-11-7	3	3	3	3	1	0	2	0	0	1	1	8
131	Isothiocyanatomethane	556-61-6	2	2	2	2	1	0	0	0	1	0	1	8
132	Lead	7439-92-1	2	2	3	2	2	2	0	0	1	0	1	8

(Sheet 3 of 5)

Table 13 (Continued)

ID	Chemicals-USAEC	CAS ID	K_{ow}	W_{sol}	VP	HLC	ASP	GI	HA	HG	HS	HSW	K_{oc}	Number of Available Parameters
137	Manganese	7439-96-5	2	2	3	1	2	2	0	0	1	0	1	8
139	Mercury	7439-97-6	3	3	3	4	2	2	0	0	1	0	2	8
149	NH3 (Ammonia)	7664-41-7	3	3	2	3	2	2	0	0	1	0	1	8
151	Nickel	7440-02-0	2	2	3	2	2	2	0	0	1	0	1	8
152	Nitric Acid	7697-37-2	2	1	2	2	1	1	0	0	1	0	1	8
154	Nitrogen Oxide (NOx)	10102-44-0	1	1	2	2	2	2	0	0	1	0	1	8
156	Nitromethane	75-52-5	2	2	2	2	1	0	1	0	1	0	1	8
157	Nonanal	124-19-6	3	3	3	3	2	1	0	0	1	0	2	8
170	Phosphorus	7723-14-0	2	3	3	2	2	2	0	0	1	0	1	8
178	Selenium	7782-49-2	2	3	2	2	2	2	0	0	1	0	1	8
179	Silver	7440-22-4	2	3	2	1	2	2	0	0	1	0	1	8
182	Sulfuric Acid	7664-93-9	2	2	2	2	1	1	0	0	1	0	1	8
184	Tetryl (2,4,6-trinitrophenylmethylnitramine)	479-45-8	3	2	2	2	2	2	0	0	1	0	2	8
185	Thallium	7440-28-0	2	2	2	1	2	2	0	0	1	0	1	8
186	Thiophene	110-02-1	3	3	3	3	1	0	1	0	0	0	1	8
188	trans-2-Butenal	123-73-9	3	3	2	3	2	1	1	0	0	0	2	8
190	trans-2-Pentene	646-04-8	3	3	3	3	1	0	1	0	0	1	1	8
195	Zinc	7440-66-6	2	2	3	2	2	2	0	0	1	0	1	8
1	1,2-Dichloroethene (cis)	156-59-2	2	2	1	2	1	1	0	0	0	0	1	7
15	1-Butene	106-98-9	2	3	3	3	1	0	1	0	0	0	1	7
17	1-Chloro-2-methylbenzene	95-49-8	4	3	3	3	2	1	0	0	0	0	2	7
19	1-Hexene	592-41-6	3	3	3	3	1	0	1	0	0	0	1	7
36	2-Methylfuran	534-22-5	3	3	3	3	1	0	1	0	0	0	1	7
44	3-Methyl-1-butene	563-45-1	3	2	3	3	1	0	0	0	0	1	1	7
45	3-Methylfuran	930-27-8	2	2	2	2	1	0	1	0	0	0	1	7
61	Acetylene	74-86-2	2	2	2	1	1	0	1	0	0	0	1	7
76	Benzo(g,h,i)perylene	191-24-2	3	3	1	3	1	1	0	0	0	0	1	7
78	Benzofuran	271-89-6	2	1	2	2	1	0	1	0	0	0	1	7
79	Benzonitrile	100-47-0	3	2	3	3	1	0	1	0	0	0	1	7
96	cis-2-Butene	590-18-1	2	2	2	2	1	0	1	0	0	0	1	7
145	Methyl-vinyl ketone	78-94-4	2	2	2	2	1	0	1	0	0	0	1	7
173	Propene	115-07-1	2	1	2	2	1	0	1	0	0	0	1	7
174	Propylene	115-07-1	2	1	2	2	1	0	1	0	0	0	1	7
189	trans-2-Butene	624-64-6	2	1	2	2	1	0	1	0	0	0	1	7
6	1,2-Dichloro-3-methylbenzene	32768-54-0	2	2	2	2	1	0	0	0	0	0	1	6
18	1-Chloro-3-methylbenzene	108-41-8	3	3	3	2	1	0	0	0	0	0	1	6
29	2,5-Dimethylfuran	625-86-5	2	2	2	2	1	0	0	0	0	0	1	6
31	2-amino-9,10-anthracenedione (a) (AAQ)	117-79-3	2	2	2	2	1	0	0	0	0	0	1	6
37	2-Methylthiophene	554-14-3	2	2	3	2	1	0	0	0	0	0	1	6
41	2-Thiophenecarboxaldehyde	98-03-3	2	2	2	2	1	0	0	0	0	0	1	6
46	3-Methylthiophene	616-44-4	2	2	3	2	1	0	0	0	0	0	1	6
53	4-phenoxy-2(1H)-quinolinone	66662-28-0	1	1	1	1	1	0	0	0	0	0	1	6

(Sheet 4 of 5)

Table 13 (Concluded)

ID	Chemicals-USAEC	CAS ID	K_{ow}	W_{sol}	VP	HLC	ASP	GI	HA	HG	HS	HSW	K_{oc}	Number of Available Parameters
70	Benzanthrone (b)	82-05-3	2	2	2	2	1	0	0	0	0	0	1	6
85	Carbon Dioxide (CO2)	124-38-9	2	2	2	2	1	0	0	0	0	0	1	6
89	Carbonyl Sulfide	463-58-1	2	2	2	2	1	0	1	0	0	0	0	6
103	Dichloroacetonitrile	3018-12-0	2	1	2	2	1	0	0	0	0	0	1	6
119	Heptanal	111-71-7	2	2	2	2	1	0	0	0	0	0	1	6
124	Hexanal	66-25-1	2	2	2	2	1	0	0	0	0	0	1	6
136	Magnesium	7439-95-4	1	1	2	1	1	1	0	0	0	0	0	6
140	Methacrolein	78-85-3	2	2	2	2	1	0	0	0	0	0	1	6
143	Methylnitrite	624-91-9	2	2	2	2	1	0	0	0	0	0	1	6
159	Octanal	124-13-0	2	2	2	2	1	0	0	0	0	0	1	6
169	Phenylacetylene (Ethynyl benzene)	536-74-3	2	2	2	2	1	0	0	0	0	0	1	6
141	Methane	74-82-8	1	1	1	1	0	0	1	0	0	0	0	5
175	Propyne	74-99-7	1	1	1	1	0	0	1	0	0	0	0	5
21	1-(Methylamino)anthraquinone (Disperse Red 9)	82-38-2	1	1	1	1	0	0	0	0	0	0	0	4
22	2-(2-quinolinyl)-1H-indene-1,3-(2H)-dione	8003-22-3	1	1	1	1	0	0	0	0	0	0	0	4
23	2-(2-quinolinyl)-1,3-indandione (D & C yellow No. 11)	8003-22-3	1	1	1	1	0	0	0	0	0	0	0	4
43	3-Furaldehyde	498-60-2	1	1	1	1	0	0	0	0	0	0	0	4
101	Dibenzo(b,def)chrysene-7,14 dione (C.I. vat yellow 4)	128-66-5	1	1	1	1	0	0	0	0	0	0	0	4
155	Nitroglycerine	55-63-0	1	1	1	1	0	0	0	0	0	0	0	4
161	o-methoxy-phenyl-azo-b-naphthol (Oil Red G)	1229-55-6	1	1	1	1	0	0	0	0	0	0	0	4
163	Particulate Cyanide	57-12-5	1	1	1	1	0	0	0	0	0	0	0	4
181	Sulfur Dioxide (SO2)	7446-09-5	1	2	2	1	0	0	0	0	0	0	0	4
191	trans-3-Penten-2-one	625-33-2	1	1	1	1	0	0	0	0	0	0	0	4
87	Carbon Monoxide (CO)	630-08-0	1	0	1	0	0	0	0	0	0	0	0	2
13	1,4-Di-p-toluidinoanthraquinone (PTA) Green 3	128-80-3	1	0	0	0	0	0	0	0	0	0	0	1
105	Dimethyltrisulfide	3658-80-8	0	0	1	0	0	0	0	0	0	0	0	1
12	1,4-Diamino-2,3-dihydroanthraquinone (DDA) violet-dye mix	81-63-0	0	0	0	0	0	0	0	0	0	0	0	0
24	2,3-Butanedione	625-34-3	0	0	0	0	0	0	0	0	0	0	0	0
42	3-(phenylhydrazone)-1H-Indole-2,3-dione		0	0	0	0	0	0	0	0	0	0	0	0
48	4-1,2,4-oxadizaolin-3-one-2,5-diphenyl-delta		0	0	0	0	0	0	0	0	0	0	0	0
49	4-Amino-2,6-Dinitrotoluene (4ADNT)	19406-51-0	0	0	0	0	0	0	0	0	0	0	0	0

(Sheet 5 of 5)

Table 14
Percentage of Chemicals in the USAEC List versus Available Parameters in Database

Number of Parameters	Percentage of Chemicals
11	13.33
10	31.28
9	8.72
8	18.46
7	8.21
6	9.74
5	1.03
4	5.13
2	0.51
1	1.03
0	2.56
	100.00

Comparison of Experimental Versus Estimated Values

This section describes a comparison between measured and estimated values for water solubility and octanol-water partitioning coefficient K_{ow} of selected explosives. The estimated values were obtained with the EPI software.

Table 15 compares solubility data computed with EPI with values obtained from literature for selected explosives. For some chemicals, such as picric acid (ID = 15), the difference is very great (difference of 10,149 mg/L). Overall, estimated solubility does not compare well with values from the literature, indicating that there may be a problem with computing this parameter with EPI. Table 16 compares measured K_{ow} data with those computed with EPI. Generally, the differences between measured and estimated K_{ow} are less than the differences for solubility.

The relative mean difference (RMD) was computed for all the data in Tables 15 and 16, where

$$RMD = \frac{\sum |M - E|}{\sum M} \qquad (1)$$

Table 15
A Comparison Among Experimental and Estimated Solubility Data for Selected Explosives

ID	Chemical Name	Brannon and Pennington (2002)		PhysPro, Howard and Meylan (2000)				EPI Estimated Solubility mg/L
		Solubility mg/L at 25 °C	Source[1]	Solubility mg/L	Temperature	Type	Source[1]	
1	2,4,6-trinitrotoluene (TNT)	100.5	Ro et al.	130	20	EXP	Seidell	552.5
2	Hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX)	59.9	Banerjee et al.	59.7	25	EXP	Dannenfelser	6,062
3	Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX)	5	Glover and Hoffsommer	140	83	EXP	Ryon et al.	2,556
4	2-Amino-4,6-Dinitrotoluene (2ADNT)	*	*	*	*	*	*	1,223
5	4-Amino-2,6-Dinitrotoluene (4ADNT)	*	*	*	*	*	*	1,223
6	2,4-Diamino-6-Nitrotoluene (2,4DANT)	*	*	*	*	*	*	
7	2,6-Diamino-4-Nitrotoluene (2,6DANT)	*	*	*	*	*	*	21,430
8	2,4-Dinitrotoluene (2,4DNT)	280	Kaye	270	22	EXP	Spanggord et al.	446.2
9	2,6-Dinitrotoluene (2,6DNT)	208	Rosenblatt et al.	182	20	EST	Spanggord et al.	352.4
10	1,3,5-Trinitrobenzene (1,3,5TNB)	385	Rosenblatt et al.	278	15	EXP	Dannenfelser	1,498
11	1,3-Dinitrobenzene (1,3DNB)	533	Rosenblatt et al.	533	25	EXP	Spanggord et al.	1,366
12	Nitrobenzene (NB)	1,797	Yalkowsky and Dannenfelser	2,090	25	EXP	Banerjee et al.	1,047
13	3-5-Dinitroaniline (3,5DNA)	*	*	1,293	25	EST	Meylan et al.	1,293
14	N,2,4,6-Tetranitro-N-methylaniline (Tetryl)	80	Urbanski	74		EXP	Dannenfelser	574.9
15	2,4,6-Trinitrophenol (Picric Acid)	12,400	Rosenblatt et al.	12,700	25	EXP	Dannenfelser	2,251
16	1,2,3-Propanetriol trinitrate (Nitroglycerine)	1,950	U.S. Army Materiel Command	1,380	20	EXP	Seidell	1,305
17	Pentaerythritol tetranitrate (PETN)	2.1	Rosenblatt et al.	43	25	EXP	Rinkenback	91.41

Note: EST = estimated; EXP = experimental or measured; * = no information.
[1] The sources listed in this column are cited in the reference above the column.

M is the measured value (or literature values), and *E* is the estimated value for each chemical. The RMD for perfect agreement is 0.0; thus a high number indicates poor agreement between estimated and measured values. The RMD for solubility was 1.30, and the RMD for K_{ow} was 0.50.

Table 16
A Comparison Between Experimental and Estimated K_{ow} (mL/mL) Data for Selected Explosives

ID	Chemical Name	Experimental Data[1]		Estimated[3]
		K_{ow}	Reference[2]	K_{ow}
1	2,4,6-trinitrotoluene (TNT)	39.81	Hansch et al.	97.72
2	Hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX)	7.41	Sangster	4.79
3	Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX)	*	*	6.61
4	2-Amino-4,6-Dinitrotoluene (2ADNT)	*	*	69.18
5	4-Amino-2,6-Dinitrotoluene (4ADNT)	*	*	69.18
6	2,4-Diamino-6-Nitrotoluene (2,4DANT)	*	*	
7	2,6-Diamino-4-Nitrotoluene (2,6DANT)	*	*	3.55
8	2,4-Dinitrotoluene (2,4DNT)	95.50	Hansch et al.	151.36
9	2,6-Dinitrotoluene (2,6DNT)	125.89	Nakgawa et al.	151.36
10	1,3,5-Trinitrobenzene (1,3,5TNB)	15.14	Hansch et al.	28.18
11	1,3-Dinitrobenzene (1,3DNB)	30.90	Hansch et al.	42.66
12	Nitrobenzene (NB)	70.79	Hansch et al.	64.57
13	3-5-Dinitroaniline (3,5DNA)	77.62	Hansch et al.	19.50
14	N,2,4,6-Tetranitro-N-methylaniline (Tetryl)			43.65
15	2,4,6-Trinitrophenol (Picric Acid)	21.38	Sangster	34.67
16	1,2,3-Propanetriol trinitrate (Nitroglycerine)	41.69	Hansch et al.	32.36
17	Pentaerythritol tetranitrate (PETN)			239.88

Note: * = no information.
[1] PhysProp Database.
[2] As cited in Howard and Meylan (2000).
[3] Estimated using EPI software.

Relative differences $(|M - E| / M)$ between measured and estimated values of Tables 15 and 16 are given in Figures 7 and 8 for solubility and K_{ow}, respectively. The x-axes of the figures show ID number of explosives as provided in Tables 15 and 16. Although there is no recommendation on the acceptable level of relative differences, the relative differences below 0.2 indicate fairly good estimated values.

The differences for these selected chemicals and properties are substantial, indicating that the estimated values may be questionable. There can be errors in measurements too, but the fact that two sources of solubility tend to be in fairly close agreement with each other but not with the estimated values casts doubts on the estimation methods. These results indicate that additional study is required before using estimation methods, especially for solubility. When measured values are not available and the estimation methods are known to produce reasonable values, then this is the only alternative for obtaining parameters required for risk characterization. In such cases, it would be beneficial to have some idea of the range of error so that uncertainty can be included in the analysis.

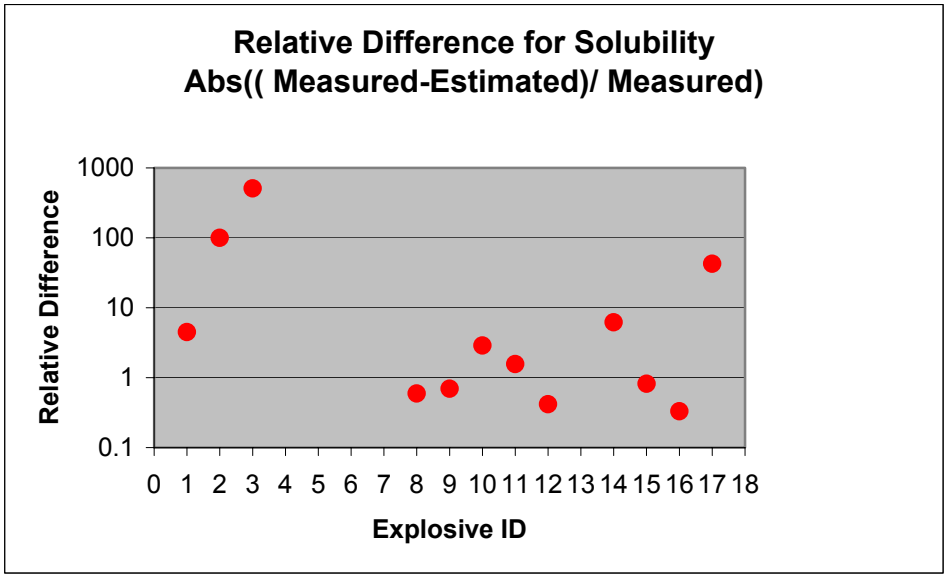


Figure 7. Relative differences of selected explosives for water solubility (explosive IDs given in Tables 15 and 16)

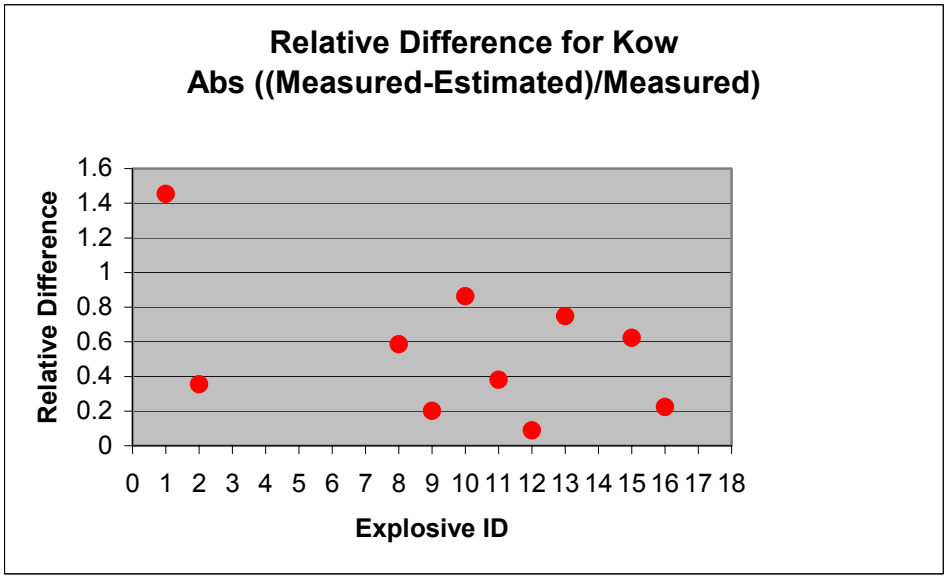


Figure 8. Relative differences of selected explosives for K_{ow} (explosive IDs given in Tables 15 and 16)

6 Summary and Conclusions

Sources of physicochemical and toxicological property data were identified that contained data specific in whole or in part to chemicals associated with military ranges. The selected data sources were from FRAMES, CHPPM, RAIS, PhysProp, and Mackay, Shiu, and Ma (2000). These data were integrated into a single Microsoft Access 2000 database. A database-user interface was developed to allow for easy comparison of physicochemical properties among the individual data sources and the display of toxicological data for these chemicals. The database is very flexible, can be updated easily, and has several useful options including printing each page of data or each cited reference. The resulting database has applications for exposure and effects assessment for risk characterization of chemicals associated with munitions and their associated emissions.

The user interface allows the user to compare the physicochemical properties of aqueous skin permeability, K_{ow}, K_{oc}, GI absorption fraction-insoluble, half-life in air, half-life in groundwater, half-life in soil, half-life in surface water, Henry's law constant, vapor pressure, and water solubility among the various data sources. The interface computes and displays the minimum, maximum, and average of the physicochemical properties. The interface also displays the toxicological properties ingestion reference dose, inhalation reference dose, threshold limit value/time-weighted average, short-term exposure levels, ingestion minimal risk levels and duration, inhalation minimal risk levels and duration, emergency response planning guidelines, Levels 1-3, acute exposure guideline Level 1, minimum contaminant levels, minimum contaminant level goals, oral cancer slope factor, and inhalation cancer slope factor. The interface allows the user to identify data gaps in physicochemical properties or toxicological benchmarks and where wide disparity among the various data sources may warrant further investigation.

Sample comparisons between measured and estimated properties indicated significant differences. In general, the differences between measured and estimated K_{ow} values were smaller compared to the differences in solubility data. Overall, the differences for these selected chemicals are substantial, indicating that either the estimated values are questionable or there may be problems with the measurement methods for the properties of the selected chemicals. These results indicate that additional study is required before using estimation methods particularly for solubility. Because of these concerns, it is preferable to have experimental (measured) chemical properties. However, measured data for many of the chemicals of interest to the Army and military are either not available or difficult to obtain. The experimental work is expensive and time-consuming. In

addition, new chemicals of concerns are being found for which properties needed for risk assessment studies are not available.

The database is limited to 11 primary properties since measured and reliable values for other properties were not available. There are techniques to estimate other properties, but as described previously, the estimated data may not be accurate. An analysis of the availability of properties in the database indicated that only 13 percent of chemicals in the list have data for all 11 properties; 30 percent of chemicals have data only for 10 properties; and 3 percent of chemicals in the list do not have any property values in the database. In general, significant gaps exist among the half-life data, especially for half-lives in groundwater, soil, and surface water, and also in toxicity data provided by CHPPM.

A number of additional tasks should be undertaken to further advance the database for short-term and long-term use:

- The foremost task should be to incorporate the half-life data of Appendix A into the database while at the same time searching additional literature to fill gaps in this type of data.

- Additionally, other data sources for all physicochemical and toxicological parameters should be sought and added to the database as appropriate and as they become available.

- Experimental measurements should be undertaken for the chemicals that are found most commonly on ranges and that have the greatest data gaps.

- Information for other physicochemical parameters, such as the transfer to food factors shown in Table 12, should be compiled or estimated.

- Existing parameter estimation techniques need to be explored more fully to find out which methods provide the greatest accuracy and to determine the degree of error associated with the methods. To accomplish this, it is recommended that all of the chemicals in the database be processed through all the commonly available estimation methods and compared with measured values.

- Recent advances in computational methods for estimating parameters should be explored.

References

Boethling, R. S., and Mackay, D., ed. (1999). *Handbook of property estimation methods for chemicals: Environmental and health sciences.* CRC, Boca Raton, FL, USA.

Brannon, J. M., and Pennington, J. C. (2002). "Environmental fate and transport process descriptors for explosives," ERDC/EL TR-02-10, U.S. Army Engineer Research and Development Center, Vicksburg, MS.

Howard, P. H. (2000). "Editorial note, celebrating QSARs," *Environmental Toxicology and Chemistry, an International Journal,* Society of Environmental Toxicology and Chemistry (SETAC), Pensacola, FL, USA, 19(3), 527.

Howard, P. H., and Meylan, W. M. (1997). "Prediction of physical properties, transport, and degradation for environmental fate and exposure assessments." *Quantitative structure-activity relationships in environmental science.* G. Schuurmann, ed., Society of Environmental Toxicology and Chemistry (SETAC), Pensacola, FL, USA, 7, 185-205.

Howard, P., and Meylan, W. (2000). "User's guide for the PHYSPROP© DATABASE ISIS™/Base Version January 2000," Syracuse Research Corporation, Environmental Science Center, North Syracuse, NY.

Lyman, W. J., Reehl, W. F., and Rosenblatt, D. H. (1990). *Handbook of chemical property estimation methods: Environmental behavior of organic compounds.* American Chemical Society, Washington, DC, USA.

Mackay, D., Shiu, W., and Ma, K. (2000). *Physical-chemical properties and environmental fate and degradation handbook.* CRCnetBASE Chapman & Hall, CRC Press, Boca Raton, FL (CD-ROM).

Miyares, P. H., and Jenkins, T. F. (2000). "Estimating the half-lives of key components of the chemical vapor signature of land mines," ERDC/CRREL TR-00-17, U.S. Army Engineer Research and Development Center, Hanover, NH.

Strenge, D. L., and Peterson, S. R. (1989). "Chemical data bases for the Multimedia Environmental Pollutant Assessment System (MEPAS): Version 1," PNL-7145, Pacific Northwest National Laboratory, Richland, WA.

U.S. Environmental Protection Agency. "ASTER," Office of Research and Development, National Health and Environmental Effect Research Laboratory, Mid-Continent Ecology Division (MED), Duluth, MN. (http://www.epa.gov/med/databases/aster.htm)

Zakikhani, M., Dortch, M. S., McGrath, C. J., Fredrickson, H. L., and Gerald, J. (2001). "Physicochemical parameters for chemicals associated with fate and transport of munitions," *Boston 2001*, presented at the Geological Society of America, Boston, MA, November 1-10, 2001. 22.

Appendix A
Additional Half-Life Data

In addition to the half-life data provided in the database, other data on half-lives were collected and are presented in this appendix. However, the data in this appendix are not included in the database since there are significant gaps (missing data) especially for the half-lives in groundwater, surface water, and soil. These data may be included in future versions of the database.

Table A1
Additional Half-Life Data

ID	Chemicals-USAEC	CAS ID	State	Ref-State[1]	Half-Life			
					Air	Groundwater	Soil	Surface Water
1	1,2-Dichloroethene (cis)							
2	1,2-Dichloroethene (trans)							
3	(1,2-dichloroethyl) benzene	1074-11-9			4-6 hours (66)			6 days (67)
4	1,2,4-Trimethylbenzene	95-63-6	L	HS	6 hours - 0.5 day (10)			3.4 hours= river (31)
5	1,2-Dichlorethane	107-06-2	L	HS	1 month (36)			several hours to 10 days (36)
6	1,2-Dichloro-3-methylbenzene	32768-54-0						
7	1,2-Dichloroethene (cis/trans MIXTURE)	540-59-0	L	HS	73 days (4)	13-48 weeks (22)		100 days - 400 days (5)
8	1,3,5-Trimethylbenzene (MESITYLENE)	108-67-8	L	HS	0.3 day (9)			
9	1,3,5-Trinitrobenzene	99-35-4			34 years(5)			23 days (68)
10	1,3-Butadiene	106-99-0	G	HS	0.2 day (9)			
11	1,3-Dinitrobenzene	99-65-0			34 years (29)			1 day (4)
12	1,4-Diamino-2,3-dihydroanthraquinone (DDA) violet-dye mix	81-63-0						
13	1,4-Di-p-toluidinoanthraquinone (PTA) Green 3	128-80-3						
14	1-Butanol	71-36-3	L	HS	1.9 days (9)			4.1 days= river;44.5 days= pond (23)
15	1-Butene	106-98-9	G	HS	0.5 day (9)			
16	Isobutylene	115-11-7	L	HS	0.3 day (9)			
7	1-Chloro-2-methylbenzene	95-49-8	L	HS				
18	1-Chloro-3-methylbenzene	108-41-8	L	CHRIS				
19	1-Hexene	592-41-6	L	HS	0.4 day (9)			
20	1-Pentene	109-67-1	L	HS	0.5 day (9)			
21	1-(Methylamino) anthraquinone (Disperse Red 9)	82-38-2						
22	2-(2-quinolinyl)-1H-indene-1,3-(2H)-dione	8003-22-3						
23	2-(2-quinolinyl)-1,3-indandione (D & C yellow no.	8003-22-3						
24	2,3-Butanedione	625-34-3						
25	2,3,7,8-Tetrachlorodibenzo-p-Dioxin	1746-01-6	S, L, G	HS	8.3 days (45)		12 years (45)	32 days to 16 days (6)
26	2,4,6-Trinitrotoluene (TNT)	118-96-7						
27	2,4-Dinitrotoluene (DNT; 2,4-DNT)	121-14-2						5 days (69)
28	2,6-Dinitrotoluene (2,6-DNT)	606-20-2			3-10 hours (69)			1.03 days (68)
29	2,5-Dimethylfuran	625-86-5	S					

(Sheet 1 of 6)

Note: Numbers in parentheses are a reference ID number; details for each reference ID citation are given in Table A2 .
[1] HS = Hazardous Substances Database; CHRIS = Chemical Hazard Response Information System.

Table A1 (Continued)

ID	Chemicals-USAEC	CAS ID	State	Ref-State[1]	Half-Life			
					Air	Groundwater	Soil	Surface Water
30	2-Amino-4,6-Dinitrotoluene	35572-78-2						
31	2-amino-9,10-anthracenedione (a) (AAQ)	117-79-3	s, (needles)	HS				
32	2-Butanone	78-93-3	L	HS	14 days (9)			15 hours (2)
33	2-Furaldehyde	98-01-1	L	HS				
34	2-Heptanone	110-43-0	L	HS	1.9 days (9)			
35	2-Methyl-1-butene	563-46-2	L	HS				
36	2-Methylfuran	534-22-5						
37	2-Methylthiophene	554-14-3						
38	2-Nitrotoluene (ONT)	88-72-2			22.9 days (9)			11 minutes (68)
39	2-Pentanone	107-87-9	L	HS	3.3 days (9)			
40	2-Propanol	67-63-0	L	HS	1-several days (50)			5.4 days (71)
41	2-Thiophenecarboxaldehyde	98-03-3						
42	3-(phenylhydrazone)-1H-Indole-2,3-dione							
43	3-Furaldehyde	498-60-2						
44	3-Methyl-1-butene	563-45-1	L or G	HS				
45	3-Methylfuran	930-27-8			0.2 day (9)			
46	3-Methylthiophene	616-44-4						
47	3-Nitrotoluene	99-08-1			16.9 days (9)			2.6 hours (68)
48	4-1,2,4-oxadizaolin-3-one-2,5-diphenyl-delta							
49	4-Amino-2,6-Dinitrotoluene (4ADNT)	19406-51-0						
50	4-Ethyltoluene	622-96-8			1.3 days (9)			
51	4-Methyl-2-Pentanone	108-10-1	L	HS	16-17 hours (18)			15-33 hours (half-time) (18)
52	4-Nitrotoluene	99-99-0						
53	4-phenoxy-2(1H)-quinolinone	66662-28-0						
54	Acenaphthene	83-32-9			0.2 day (9)			
55	Acenaphthylene	208-96-8	S?	HS			12 to 121 days (46)	4 days= river; 184 days= pond (71)
56	Acetaldehyde	75-07-0	L @ <69 °F	HS	1 day (9)			3 hours (53)
57	Acetic Acid	64-19-7	L @ >62°F	HS	45.58 years (8)			
58	Acetone	67-64-1	L	HS	71 days (9)			13.7 hours (21)
59	Acetonitrile	75-05-8	L	HS	0.6 day to 20 days (11)			11 days= pond; 6 days= river (12)
60	Acetophenone	98-86-2	L	HS	5.9 days (9)	32 days (63)		8 days+ river; 4.5 days= pond (62)
61	Acetylene	74-86-2	G@ 15 °C	HS	19.7 days (9)			
62	Acrolein	107-02-8	L	HS	0.8 day (9)		14 days (71)	1-3 days (1)
63	Acrylonitrile	107-13-1	L	HS	4 days (9)			1-6 days (12)

(Sheet 2 of 6)

Table A1 (Continued)

ID	Chemicals-USAEC	CAS ID	State	Ref-State[1]	Half-Life			
					Air	Groundwater	Soil	Surface Water
64	Aluminum	7429-90-5	S	HS				
65	Anthracene	120-12-7			0.1 day (9)			45 minutes (70)
66	Antimony	7440-36-0	S	HZ	30 days (2)			
67	Arsenic	7440-38-2	S	HS				
68	Barium	7440-39-3	S	HS				
69	Benzaldehyde	100-52-7	L	HS	1.2 days (9)			37 hours = river; 17 days= pond (34)
70	Benzanthrone (b)	82-05-3						
71	Benzene	71-43-2	L	HS	13 days (9)			8.8 - 673 days (65)
72	Benzo(a)anthracene	56-55-3						0.59 hour (70)
73	Benzo(a)pyrene	50-32-8						0.54 hour (70)
74	Benzo(b)fluoranthene	205-99-2						
75	Benzo(e)pyrene	192-97-2						
76	Benzo(g,h,i)perylene	191-24-2						
77	Benzo(k)fluoranthene	207-08-9						
78	Benzofuran	271-89-6	L	HS	0.4 day (9)			
79	Benzonitrile	100-47-0	L	HS	48.6 days (9)			
80	Beryllium	7440-41-7	S	HS				>200 days (32)
81	Bis(2-ethylhexyl)phthalate	117-81-7	L	HS	16.4 hours (40)			2-3 weeks (38)
82	Butanal	123-72-8	L	HS	0.7 day (9)			9 hours= river; 4.1 hours= pond (24)
83	Cadmium	7440-43-9	S	HS				
84	Calcium	7440-70-2						
85	Carbon Dioxide (CO2)	124-38-9	G or L	HS				
86	Carbon Disulfide	75-15-0	L	HS	12 days (14)		1.5 days (71)	2.6 hours (14)
87	Carbon Monoxide (CO)	630-08-0	G	HS				
88	Carbon tetrachloride	56-23-5	L	HS	366 years (9)	3-300 days (48)	no data available (48)	6 - 12 months (3)
89	Carbonyl Sulfide	463-58-1	G or L	HS	2 years (15)			2.3 hours= river (15)
90	Chlorobenzene	108-90-7	L	HS	20.8 days		0.3 day= 1 cm deep; 12.6 days = 10 cm deep (27)	8 hours= river; 1-12 hours= stream (16)
91	Chloroethene (Vinyl chloride)							
92	Chloroform	67-66-3	L	HS	71 days (9)			
93	Chloromethane	74-87-3			19.7 days (9)			10.6 days (6)
94	Chromium	7440-47-3	S	HS				
95	Chrysene	218-01-9						4.4 hours (70)
96	cis-2-Butene	590-18-1	G	HS	0.3 day (9)			

Table A1 (Continued)

ID	Chemicals-USAEC	CAS ID	State	Ref-State[1]	Half-Life			
					Air	Groundwater	Soil	Surface Water
97	Cl2 (a)	7782-50-5	G	HS				
98	Cobalt	7440-48-4	S	HS				
99	Copper	7440-50-8	S	HS				
100	Dibenz(a,h)anthracene	53-70-3						
101	Dibenzo(b,def)chrysene-7,14 dione (C.I. vat yellow 4)	128-66-5						
102	Dibutyl Phthalate	84-74-2	L	HS	14 hours (7)			3-5 days to 3 weeks (58)
103	Dichloroacetonitrile	3018-12-0						
104	Dichlorodiflouromethane	75-71-8	G	HS	16044 days (9)			
105	Dimethyltrisulfide	3658-80-8						
106	Dioctyl Phthalate	117-81-7	L	HS	16.4 hours (40)			2-3 weeks (38)
107	Dioxin TEQ (c)	1746-01-6	S, L, G	HS	8.3 days (45)		12 years (45)	32 days to 16 days (6)
108	Diphenylamine	122-39-4						
109	Ethane	74-84-0	G	HS	59.9 days (9)			1.5 hours = river; 1.9 days= pond (64)
110	Ethanol	64-17-5	L	HS	4.9 days (9)			6 days (49)
111	Ethylbenzene	100-41-4	L	HS	2.3 days (9)			several days to 2 weeks (33)
112	Ethylchloride	75-00-3	L	HS	41.1 days (9)	38 days (71)		1.1 to 5.6 days (52)
113	Ethylene	74-85-1	G	HS	1.9 days (9)			
114	Fluoranthene	206-44-0						
115	Fluorene	86-73-7	S	HS	1.2 days (9)		2-64 days (59)	15 hours = river; 167 hours = pond (71)
116	Formaldehyde	50-00-0			1.7 days(9)			
117	Furan	110-00-9	L	HS	0.4 day (9)			
118	HCl	7647-01-0	L	HS				
119	Heptanal	111-71-7	L	HS				
120	Hexachlorobenzene	118-74-1	S	HS	2 years (39)		1530 days (39)	ca 8 hrs (39)
121	Hexachlorobutadiene	87-68-3	L	HS	1.6 months (60)	30-300 days (60)		3-30 days= river; 30-300= lake (3)
122	Hexachlorocyclopentadiene	77-47-4	L	HS	2 months - 1 hour (57)	several hours to 2-3 weeks (57)	hours to weeks (57)	2-8.5 minutes to 37 days (57)
123	Hexachloroethane	67-72-1	S	HS	30 years (51)			15 hours (51)
124	Hexanal	66-25-1	L	HS				
125	Hexane	110-54-3	L	HS	2.9 days (9)			<3 hours= river; 6.8 days= pond (25)
126	HMX	2691-41-0						
127	Hydrogen Cyanide	74-90-8			0.7 day (9)			
128	i-Butane (isobutane)	75-28-5			6.9 days (9)			
129	i-Butene (isobutene/E-butylene)	115-11-7	L	HS	0.3 day (9)			

(Sheet 4 of 6)

Table A1 (Continued)

ID	Chemicals-USAEC	CAS ID	State	Ref-State[1]	Half-Life			
					Air	Groundwater	Soil	Surface Water
130	Indeno(1,2,3-cd)pyrene	193-39-5						
131	Isothiocyanatomethane	556-61-6	S	HS				
132	Lead	7439-92-1	S	HS				
133	Xylene (mixed isomers)							
134	m-Xylene (meta-xylene)							
135	p-Xylene (para-xylene)							
136	Magnesium	7439-95-4	S	HS				
137	Manganese	7439-96-5	S	HS				
138	m-Dichlorobenzene	541-73-1	L	HS	22.3 days (9)			3.1 hours (47)
139	Mercury	7439-97-6	L	HS				
140	Methacrolein							
141	Methane	74-82-8			1908 days (9)			
142	Methylene Chloride	75-09-2	L	HS	0.3 day (9)			21 minutes (17)
143	Methylnitrite	624-91-9						
144	Methyl-t-butylether (MTBE)	1634-04-4	L	HS	5.7 days (9)			2.5 hours= stream; 9.5 hours= river; 137 days= lake (44)
145	Methyl-vinyl Ketone	78-94-4			0.9 day (9)			
146	Naphthalene	91-20-3	S	HS	0.7 day (9)	3 to 18 days (71)		71 hours (70)
147	n-Butane	106-97-8	G	HS	6.3 days (9)			
148	n-Decane	124-18-5	L	HS	1.4 days (9)			
149	NH3 (Ammonia)	7664-41-7						
150	n-Hexane	110-54-3	L	HS	2.9 days (9)			<3 hours= river; 6.8 days= pond (25)
151	Nickel	7440-02-0	S	HS				
152	Nitric Acid	7697-37-2						
153	Nitrobenzene	98-95-3			5.9 days (9)			0.3 day (19)
154	Nitrogen Oxide (NOx)	10102-44-0	G	HS				
155	Nitroglycerine	55-63-0						
156	Nitromethane	75-52-5	L	HS	1.7 days (9)		19 days= 10 cm (26)	28.7 hours = river; 13 days= pond (54)
157	Nonanal	124-19-6						
158	OCDD (1,2,3,4,6,7,8,9-OCDD)	3268-87-9						
159	Octanal	124-13-0	L	HS				
160	o-Dichlorobenzene	95-50-1	L	HS	38.2 days (9)	30-300 days (62)		4.4 hours to 30 days (62)
161	o-methoxy-phenyl-azo-b-naphthol (Oil Red G)	1229-55-6						
162	o-Xylene (ortho-xylene)	95-47-6	L	HS	1.2 days (9)			
163	Particulate Cyanide							
164	p-Dichlorobenzene (para-Dichlorobenzene)	106-46-7	S	HS	50.1 days (9)			4.3 hours (35)

Table A1 (Concluded)

ID	Chemicals-USAEC	CAS ID	State	Ref-State[1]	Half-Life			
					Air	Groundwater	Soil	Surface Water
165	Pentaerythritoltetranitrate (PETN)	78-11-5						
166	Perchloroethylene	127-18-4	L	HS	96.1 days (9)			3 hours – 14 weeks (43)
167	Phenanthrene	85-01-8	S	HS	0.5 day (9)			8.4 hours (70)
168	Phenol	108-95-2	S	HS	0.61 day (9)		<5 days (28)	100 days (6)
169	Phenylacetylene (Ethynyl benzene)	536-74-3						
170	Phosphorus	7723-14-0	S	HS				
171	Propanal	123-38-6	L	HS	0.8 day (9)			11 hours = river; 5 days= pond (71)
172	Propane	74-98-6	G	HS	14 days (9)			
173	Propene	115-07-1	G	HS	0.6 days (9)			
174	Propylene	115-07-1	G	HS	0.6 days (9)			
175	Propyne	74-99-7			2.7 days (9)			
176	Pyrene	129-00-0						0.6 hour (70)
177	RDX	121-82-4			1.5 hours (4)			9 – 13 hours (4)
178	Selenium	7782-49-2	S	HS				
179	Silver	7440-22-4	S	HS				
180	Styrene (Vinyl benzene)	100-42-5	L	HS	0.3 day (9)			0.6 – 13 days (19)
181	Sulfur Dioxide (SO2)	7446-09-5	G	HS				
182	Sulfuric Acid	7664-93-9						
183	Tetrachloroethene	127-18-4	L	HS	96.1 days (9)			3 hours - 14 weeks (43)
184	Tetryl (2,4,6-trinitrophenylmethylnitramine)	479-45-8			>10 days (4)			
185	Thallium	7440-28-0						
186	Thiophene	110-02-1	L	HS	1.7 days (9)			
187	Toluene	108-88-3	L	HS	2.7 days (9)		1-7 days (20)	1-16 days to 5-6 hours (20)
188	trans-2-Butenal	123-73-9	L	HS	11 hours (41)			5 days to 18.3 days (41)
189	trans-2-Butene	624-64-6	G	HS	0.3 day (9)			
190	trans-2-Pentene	646-04-8	L	HS	0.2 day (9)			
191	trans-3-Penten-2-one	625-33-2						
192	Trichloroethylene (TCE)	79-01-6	L	HS	6.8 days (9)			10.7 – 30 months (4)
193	Trichloroflouromethane	75-69-4	L (< 23.7 °C)	HS	22920 days (9)		52-207 years (55)	6.1 hours= river (55)
194	Vinylidenechloride	75-35-4	L	HS	2 days (9)	5-6 months (30)		5.9 days= pond; 4.7 days= lake; 1.2 days= river (30)
195	Zinc	7440-66-6	S	HS				

Table A2
References for Table A1

1	Agency for Toxic Substances and Disease Registry (ATSDR). 1990. Toxicological profile for acrolein. Atlanta, GA: U.S. Department of Health and Human Services, Public Health Service. (Bowmer and Higgins 1976; Bowmer et al. 1974)
2	Agency for Toxic Substances and Disease Registry (ATSDR). 1992. Toxicological profile for antimony. Atlanta, GA: U.S. Department of Health and Human Services, Public Health Service. (Schroeder et al. 1987)
3	Agency for Toxic Substances and Disease Registry (ATSDR). 1994. Toxicological profile for hexachlorobutadiene. Atlanta, GA: U.S. Department of Health and Human Services, Public Health Service.
4	Agency for Toxic Substances and Disease Registry (ATSDR). 1995. Toxicological profile for trichloroethylene. Atlanta, GA: U.S. Department of Health and Human Services, Public Health Service.
5	Agency for Toxic Substances and Disease Registry (ATSDR). 1996. Toxicological profile for 1,3,5-trinitrobenzene. Atlanta, GA: U.S. Department of Health and Human Services, Public Health Service. (Atkinson 1985, 1987; HSDB 1994)
6	Agency for Toxic Substances and Disease Registry (ATSDR). 1998. Toxicological profile for phenol. Atlanta, GA: U.S. Department of Health and Human Services, Public Health Service. (Mill and Mabey 1985)
7	Agency for Toxic Substances and Disease Registry (ATSDR). 1999. toxicological profile for di-n-butyl phthalate. Atlanta, GA: U.S. Department of Health and Human Services, Public Health Service.
8	Anbar,M.; Neta,P.; A compilation of specific bimolecular rate constant for the reactions of hydrated electrons, hydrogen atoms and hydroxyl radical with inorganic and organic compounds in aqueous solution.; Int. J. of appl. Radiation and isotopes.; 18:493-523.; 1967
9	Atkinson, R (1989) Atkinson, R.; Kinetics and Mechanisms of the Gas-Phase Reactions of the Hydroxyl Radical with Organic Compounds.; Journal of Physical and Chemical Reference Data. Monograph No. 1.; 1989
10	Atkinson, R.; Kinetics and Mechanisms of the Gas-Phase Reactions of the Hydroxyl Radical with Organic Compounds.; Journal of Physical and Chemical Reference Data. Monograph No. 1.; 1989
11	EPA envirofacts; chemical summary for Acetonitrile; EPA 749-F-94-004a; August 1994 (CHEMFATE 1994) (U.S. EPA 1985)
12	EPA envirofacts; chemical summary for Acetonitrile; EPA 749-F-94-004a; August 1994 (U.S. EPA 1985)
13	EPA envirofacts; chemical summary for Acrylonitrile; EPA 749-F-95-001a; December 1994 (U.S. EPA 1985)
14	EPA envirofacts; chemical summary for Carbon Disulfide; EPA 749-F-94-008a; August 1994 (ATSDR 1992) (U.S. EPA 1986)
15	EPA envirofacts; chemical summary for Carbonyl Sulfide; EPA 749-F-94-009a; August 1994 (HSDB 1994)
16	EPA envirofacts; chemical summary for Chlorobenzene; EPA 749-F-95-007a;January 1995 (U.S. EPA 1988; Howard 1989)
17	EPA envirofacts; chemical summary for dichloromethane; EPA 749-F-94-018a; August 1994 (HSDB 1994)
18	EPA envirofacts; chemical summary for methyl isobutyl ketone; 749-F-94-009a; September 1994
19	EPA envirofacts; chemical summary for nitrobenzene; EPA 749-F-95-015a; February 1995 (HSDB 1994)
20	EPA envirofacts; chemical summary for Toluene; EPA 749-F-94-021a; August 1994
21	Graedel,T.E.; chemical compounds in the atmosphere.; New York,NY: Academic press. PP.440.; 1978
22	http://chem.sis.nlm.nih.gov/chemidplus/detail_frame.html?DetailIndex=1&DetailCount=1
23	http://chem.sis.nlm.nih.gov/chemidplus/detail_frame.html?DetailIndex=1&DetailCount=2
24	http://chem.sis.nlm.nih.gov/chemidplus/detail_frame.html?DetailIndex=1&DetailCount=29
25	http://chem.sis.nlm.nih.gov/chemidplus/detail_frame.html?DetailIndex=1&DetailCount=32
26	http://chem.sis.nlm.nih.gov/chemidplus/detail_frame.html?DetailIndex=1&DetailCount=33
27	http://chem.sis.nlm.nih.gov/chemidplus/detail_frame.html?DetailIndex=1&DetailCount=34
28	http://chem.sis.nlm.nih.gov/chemidplus/detail_frame.html?DetailIndex=1&DetailCount=44
29	http://chem.sis.nlm.nih.gov/chemidplus/detail_frame.html?DetailIndex=1&DetailCount=5
30	http://chem.sis.nlm.nih.gov/chemidplus/detail_frame.html?DetailIndex=1&DetailCount=58
31	http://chem.sis.nlm.nih.gov/chemidplus/detail_frame.html?DetailIndex=1&DetailCount=9
32	http://www.sonic.net/kryptox/medicine/pfpc/jones.txt
33	http://www.speclab.com/compound/c100414.htm
34	http://www.speclab.com/compound/c100527.htm
35	http://www.speclab.com/compound/c106467.htm
36	http://www.speclab.com/compound/c107062.htm
37	http://www.speclab.com/compound/c111717.htm
38	http://www.speclab.com/compound/c117817.htm
39	http://www.speclab.com/compound/c118741.htm
40	http://www.speclab.com/compound/c123728.htm
41	http://www.speclab.com/compound/c123739.htm
42	http://www.speclab.com/compound/c124196.htm
43	http://www.speclab.com/compound/c127184.htm
44	http://www.speclab.com/compound/c1634044.htm
45	http://www.speclab.com/compound/c1746016.htm
46	http://www.speclab.com/compound/c208968.htm

(Continued)

Table A2 (Concluded)	
47	http://www.speclab.com/compound/c541731.htm
48	http://www.speclab.com/compound/c56235.htm
49	http://www.speclab.com/compound/c64175.htm
50	http://www.speclab.com/compound/c67630.htm
51	http://www.speclab.com/compound/c67721.htm
52	http://www.speclab.com/compound/c75003.htm
53	http://www.speclab.com/compound/c75070.htm
54	http://www.speclab.com/compound/c75525.htm
55	http://www.speclab.com/compound/c75694.htm
56	http://www.speclab.com/compound/c75718.htm
57	http://www.speclab.com/compound/c77474.htm
58	http://www.speclab.com/compound/c84742.htm
59	http://www.speclab.com/compound/c86737.htm
60	http://www.speclab.com/compound/c87683.htm
61	http://www.speclab.com/compound/c91203.htm
62	http://www.speclab.com/compound/c95501.htm
63	http://www.speclab.com/compound/c98862.htm
64	http://www.toxnet.nlm.nih.gov/cgi-bin/sis/search/f?./temp/~BAAWxaOBz:1
65	Hustert,K.; Mansour,M.; Parlar,H.; Korte,F.; The EPA test- a method to determine the photochemical degradation of organic compounds in aquatic systems.; chemosphere.; 10:995-8.; 1981
66	Korte, F.; Klein, W.; Degradation of Benzene in the Environment.; Ecotoxicol. Environ. SAF.; 6:311-27.; 1982
67	Lee,R.F.; Ryan,C.; Microbial Degradation of organochlorine compounds in esturine waters and sediments.; In: EPA-600/9-79-012. Microbial degradation of pollutants in marine environments. Bourquin, A.W., & Pritchard, P.H., Eds. Gulf Breeze, FL:U.S. EPA. PP>443-50.; 1979
68	Simmons,M.S.; Zepp,R.G.; Influence of humic substances on photolysis of nitroaromatic compounds in aqueous systems.; water res.; 20:899-904; 1986
69	Spanggord,R.J.; Mill,T.; Chou,T.W.; Mabey,W.R.; Smith,J.H.; Lee,S.; Environmental fate studies on certain munitions wastewater constituents. Final report, Phase 1- Literature review.; SRI project no. LSU-7934. Contract no. DAMD 17-78-C-8081. Fort Detrick, MD: U.S. Army Medical Res.& Develop. Command.; 1980
70	Zepp,R.G.; Schlotzhauer,P.F.; photoreactivity of selected aromatic hydrocarbons in water.; IN: polynuclear aromatic hydrocarbons. Jones, P.W., & Leber, P., Eds., Ann Arbor,MI: ann arbor science publishers, inc. PP> 141-58.; 1979

Appendix B
Toxicity Information/Database for Range-Specific Substances

U.S. Army Center for Health Promotion and Preventive Medicine

USCHPPM

TOXICOLOGY STUDY NO.87-MA-6943-01
TOXICITY INFORMATION/
DATABASE FOR
RANGE-SPECIFIC SUBSTANCES
MAY 2001 – SEPTEMBER 2001

Prepared by
Health Effects Research Program
Directorate of Toxicology

Toxicology Study No. 87-MA-6943-01
Approved for Public Release; Distribution Unlimited

Readiness Thru Health

TOXICOLOGY STUDY NO.87-MA-6943-01
TOXICITY INFORMATION/
DATABASE FOR
RANGE-SPECIFIC SUBSTANCES
MAY 2001 – SEPTEMBER 2001

Approved for public release; distribution is unlimited.

EXECUTIVE SUMMARY
TOXICOLOGY STUDY NO. 87-MA-6943-01
TOXICITY INFORMATION/
DATABASE FOR
RANGE-SPECIFIC SUBSTANCES
MAY 2001 – SEPTEMBER 2001

Many training activities at U.S. Army installations involve the use of pyrotechnic, explosive, and incendiary compounds. Residues of these substances have been associated with training activities and found in soil, air, and surface water samples. Current environmental regulation requires extensive assessment of human health and environmental related effects from exposure to substances in soil, surface water and ground water. It is most efficient to evaluate the potential for exposure, effects, and transport of these training related substances before environmental releases occur. This requires knowledge of the toxicological effects of substances of potential concern. The purpose of this effort was to develop a database of toxicity benchmark values of substances related to training activities for use as an indicator of the availability of toxicity data. Toxicity benchmarks were available for more than 120 substances (Appendix B); often more than one benchmark was found. No values were available for 70 substances, suggesting few toxicity data were available or that the current jurisdictions found no use in deriving benchmark values for those specific substances. These data provide the basis for prioritizing the need for further study of several compounds. However, other factors of exposure must be recognized in any prioritization scheme. The amount used, environmental persistence, and fate and transport issues must also be considered in directing future research efforts. It is recommended that a more focused toxicity profile be conducted for each substance where data are lacking so that a more accurate characterization can be made.

Sponsor

U.S. Army Environmental Center
Installation Restoration Program
Aberdeen Proving Ground, MD 21010

Study Title

Toxicity Information/Database For
Range-Specific Substances

Data Requirement

Not Applicable

Authors

Christopher J. Salice, Howard T. Bausum, Mark S. Johnson

Study Completed

September 2001

Performing Laboratory

U.S. Army Center for Health Promotion and Preventive Medicine
ATTN: MCHB-TS-THE
Aberdeen Proving Ground, MD 21010-5403

Submitted By:

U.S. Army Center for Health Promotion and Preventive Medicine
Health Effects Research Program
ATTN: MCHB-TS-THE
Aberdeen Proving Ground, MD 21010-5403
(410) 436-3980

Prepared By:

Christopher J. Salice, Ph.D. (*candidate)* Biologist, HERP	Date
Howard T. Bausum, Ph.D. Biologist, HERP	Date
Mark S. Johnson, Ph.D. Biologist, HERP	Date

Approved By:

Michael A. Major, Ph.D, DABT Program Manager Health Effects Research	Date

TABLE OF CONTENTS

TOXICOLOGY STUDY NO. 87-MA-6943-01
TOXICITY INFORMATION/DATABASE FOR
RANGE-SPECIFIC SUBSTANCES
MAY 2001 – SEPTEMBER 2001

1. REFERENCES. See Appendix A for a listing of references.

2. AUTHORITY. This research was completed as part of the Army Environmental Center's (AEC) efforts to determine the state of information needed to conduct training activities in a manner consistent with environmental sustainability.

3. PURPOSE. To develop a database of toxicity benchmark values of substances related to training activities for use as an indicator of the availability of toxicity data.

4. GENERAL BACKGROUND.

a. Essential National Defense strategies require that the armed forces be in a ready, trained state. Maintaining training activities at U.S. Army installations is crucial for the military to function at such a readiness state. Military personnel involved in training exercises may be exposed to substances that may compromise their health. Moreover, land capable of supporting training activities must also maintain vital natural resources, and therefore must be used in an environmentally sustainable manner.

b. Current environmental regulation requires extensive assessment of human health and environmental effects arising from exposure to substances in soil, surface water and ground water. Applied retroactively, these assessment efforts are costly and highly uncertain. It is more efficient to evaluate the potential for exposure, effects, and transport of these training related substances before environmental releases occur, thereby saving resources, money, and sustaining the health of those potentially exposed. In an effort to support this preventive approach, the AEC has asked that U.S. Army Center for Health Promotion and Preventive Medicine (USACHPPM) assemble toxicity data on military-important substances that may be encountered during training exercises. The purpose is to determine the extent of toxicological information available in order to direct and focus efforts where data are lacking. The Engineering Research Development Center (ERDC), Environmental Laboratory (formerly Waterways Experiment Station) has been tasked to develop a database of fate and transport information regarding the tentatively identified compounds from training activities. The USACHPPM in coordination with ERDC has been tasked to evaluate the extent of toxicity information for these substances.

c. Given the extensive list, a complete compound-by-compound literature review was not feasible. Therefore, it was decided that a compilation of existing toxicity benchmarks would provide a reasonable indication that sufficient toxicity information exists for those compounds with published values, and is lacking for those without. It

was the intention of the AEC and USACHPPM representatives that this work would determine where data gaps exist and where to focus additional resources.

5. METHODS.

a. Ms. Tamara Barker representing AEC provided USACHPPM a list of 191 tentatively identified compounds. For each chemical on this list, several databases were searched for the following applicable toxicity benchmarks:

Threshold Limit Values (TLVs),
Short-Term Exposure Limits (STELs),
Reference Doses (RfDs),
Reference Concentrations (RfCs),
Cancer slope factors,
Emergency Response Planning Guidelines (ERPGs),
Acute Emergency Guideline Levels (AEGLs),
Minimum Risk Levels (MRLs),
Continuous Exposure Guideline Levels (CEGLs),
Emergency Exposure Guideline Levels (EEGLs),
Maximum Contaminant Levels (MCLs),
Immediately Dangerous to Life and Health (IDLHs), and
Permissible Exposure Level (PELs).

b. These benchmarks were developed by the American Conference of Governmental Hygienist (ACGIH), (reference 1), the U.S. Environmental Protection Agency (EPA), (reference 2-5), American Industrial Hygiene Association (AIHA), (reference 6), Agency for Toxic Substances and Disease Registry (ATSDR),(reference 7), National Research Council (NRC), Committee on Toxicology (reference 8 and 11), and the National Institute of Occupational Safety and Health (NIOSH), (reference 9 and 10). They encompass acute, subchronic, and chronic exposures, have been developed for occupational, military, and emergency applications, and consider various human subpopulations in their derivation. No consistent methods were used in their derivation, and these benchmarks are subject to various degrees of peer review. In addition, chemical-specific properties may predispose the development of some values (e.g., airborne volatiles as RfCs, TLVs, etc., vs. solids as RfDs, MCLs, etc.).

c. Appendix B describes and defines each toxicity benchmark. Brief explanations and descriptions of the toxicity benchmarks are presented in Table 1.

Table 1. Toxicity Benchmarks searched for Tentatively Identified Compounds associated with range use.

Benchmark		Jurisdiction	Target Population	Exposure route	Comments
Threshold Limit Value Short Term Exposure Limit	TLV STEL	ACGIH	Workers	Inhalation	Developed as guidelines to protect workers in industrial scenarios.
Reference Dose	RfD	USEPA	General population	Ingestion exposures	Developed to address chronic exposures.
Reference Concentration	RfC	USEPA	General population	Inhalation exposures	Developed to address chronic inhalation exposures.
Slope Factors	Sf	USEPA	General population	Inhalation and oral	Addresses risks from exposure to carcinogens.
Emergency Response Planning Guideline	ERPG	AIHA	General population	Inhalation	1-hr values developed for emergency response planning.
Acute Exposure Guideline Level	AEGL	USEPA	General population	Inhalation	1-hr values developed for acute inhalation scenarios (similar to ERPGs).
Minimum Risk Level	MRL	ATSDR	General population	Inhalation and oral	Acute, intermediate, and chronic values.
Continuous Exposure Guideline Level	CEGLs	NRC	Military	Inhalation	For 90-d continuous exposures. Few exist.
Emergency Exposure Guideline Level	EEGL	NRC	Military	Inhalation	For acute exposures.
Maximum Contaminant Level	MCL	USEPA	General population	Oral	Developed for concentrations of substances in drinking water.
Immediately Dangerous to Life and Health	IDLH	NIOSH	Occupational	Inhalation	Developed for mask issue use.
Permissible Exposure Level	PEL	NIOSH	Occupational	Inhalation	Developed for occupational use.

6. RESULTS.

a. Literature Search. Toxicity benchmarks were available for more than 120 substances (Appendix B); often more than one benchmark was found. No values were available for 70 substances, suggesting few toxicity data were available or that the current jurisdictions found no use in deriving benchmark values for those specific substances.

b. Data Presentation. The results of the search are presented in Appendix C.

7. DISCUSSION.

a. Toxicity benchmarks exist for approximately two-thirds of the substances that were evaluated. Two reasons may account for these results. Either insufficient toxicity data were available to develop a reliable toxicity benchmark, or those exposures to these substances were determined to be insufficient for these various jurisdictions to justify the derivation of a toxicity benchmark. A likely corollary may lie in the availability of fate and transport information, since this information is often collected in concert with toxicity testing data.

b. The presence of a benchmark is a likely indicator that sufficient toxicity data exist, yet many developers use methods of extrapolation that result in exceedingly low values to compensate for an insufficient and lacking toxicity database. Therefore, the presence of a single value may not be a reliable indication that adequate toxicity information exists. However, sufficient and adequate toxicity information is likely for substances where several benchmarks were found.

c. The only benchmark that intentionally evaluated the likelihood of cancer was the Cancer Slope Factor. Since long-term animal studies are needed for a proper evaluation of the potential for cancer from exposure, relatively few studies exist. Therefore, although the presence of a value is an indication that data do exist, the lack of a value cannot be construed that a specific substance is not carcinogenic, only that no reliable chronic human or animal data exist.

d. These data provide the basis for prioritizing the need for further study of several compounds. However, other factors of exposure must be recognized in any prioritization scheme. The amount used, environmental persistence, and fate and transport issues must also be considered in directing future research efforts. It is recommended that a more focused toxicity profile be conducted for each substance where data are lacking so that a more accurate characterization can be made.

8. ACKNOWLEDGEMENTS

a. We thank Dr. Mark Dortch of the Engineering Research and Development Center for providing the funding to conduct this review. This study was funded indirectly by U.S. AEC.

_____
CHRISTOPHER J. SALICE
Biologist

APPROVED:

_____
MICHAEL A. MAJOR
Program Manager
Health Effects Research

APPENDIX A:

REFERENCES

1. American Conference of Governmental Industrial Hygienists (ACGIH). 1999. Documentation of the Threshold Limit Values and Biological Exposure Indices. American Conference of Governmental Hygienists, Inc., Cincinnati, OH.

2. United States Environmental Protection Agency (EPA). 2001. Online Integrated Risk Information System (IRIS).

3. United States Environmental Protection Agency (EPA). 2001. Online Current Drinking Water Standards.

4. United States Environmental Protection Agency, Office of Research and Development (EPA-ORD). 1997. Health Effects Assessment Summary Tables. U.S. Environmental Protection Agency, Washington, D.C.

5. United States Environmental Protection Agency, Region III (EPA). 2001. EPA Region III RBC Table. U.S. Environmental Protection Agency, Washington, D.C.

6. American Industrial Hygiene Association (AIHA). 2001. Emergency Response Planning Guidelines and Workplace Environmental Exposure Level Guides Handbook. American Industrial Hygiene Association, Fairfax, VA.

7. Agency for Toxic Substances and Disease Registry (ATSDR). 2001. Online Minimal Risk Levels for Hazardous Substances. U.S. Department of Health and Human Services, Public Health Service.

8. National Research Council, Committee on Toxicology (NRC). Acute Exposure Guideline Levels and Continuous Exposure Guideline Levels. National Academy Press, Washington, D.C.

9. National Institute for Occupational Safety and Health (NIOSH). 1988. Online OSHA PEL Project Documentation. National Institute for Occupational Safety and Health, Cincinnati, OH.

10. National Institute for Occupational Safety and Health (NIOSH). 1994. Documentation for Immediately Dangerous to Life or Health Concentrations (IDLHs). National Institute for Occupational Safety and Health, Cincinnati, OH.

11. National Research Council (NRC). 1984. Emergency and Continuous Exposure Limits for Selected Airborne Contaminants. AD-A142-133. Committee on Toxicology. National Academy Press, Washington, D.C.

APPENDIX B:

TOXICITY BENCHMARK DEFINITIONS

1.0 Acute Toxicity Benchmarks:

Several sources that provide 1-hour air values were evaluated in selecting these values. These sources included: Emergency Response Planning Guidelines (ERPGs, Levels 1-3) from the AIHA; Emergency Exposure Guidance Levels (EEGLs) from the National Academy of Sciences (NAS), NRC/Committee on Toxicology (COT); and, Acute Exposure Guideline Levels (AEGLs, Levels 1-3) from the EPA; and, Short Term Exposure Limits (STELs) from the ACGIH. Each source described above established values for a specific application. Descriptions of each are given below.

ERPGs intended for emergency planning and response operations have been developed by the AIHA. They are based on a weight-of-evidence evaluation and are reviewed at regular intervals as new information becomes available. Definitions of the three levels of ERPG values are:

- ERPG-1: The maximum airborne concentration below which it is believed nearly all individuals could be exposed for up to 1 hour without experiencing more than mild, transient adverse health effects or without perceiving a clearly defined objectionable odor.

- ERPG-2: The maximum airborne concentration below which it is believed nearly all individuals could be exposed for up to 1 hour without experiencing or developing irreversible or other serious health effects or symptoms that could impair an individual's ability to take protective action.

- ERPG-3: The maximum airborne concentration below which it is believed nearly all individuals could be exposed for up to 1 hour without experiencing or developing life-threatening health effects.

The ERPGs are intended to protect most individuals in the general population but not particularly sensitive individuals (reference 6). All populations have hyper-sensitive individuals who may show adverse effects at concentrations below these guidelines.

The AEGLs are intended to protect the general public, including sensitive sub-populations but not hypersensitive or hypersusceptible individuals (reference 8). They are derived for 30-minute, 1-hour, 4-hour, and 8-hour exposures. As with ERPGs, there are 3 levels:

- AEGL-1: The airborne concentration of a substance at or above which it is predicted that the general population (including "susceptible" but excluding "hyper-susceptible" individuals) could experience notable discomfort. Concentrations below AEGL-1 represent exposure levels that could produce mild odor, taste, or other sensory irritations.

- AEGL-2: The airborne concentration of a substance at or above which it is predicted that the general population (including "susceptible" but excluding "hyper-susceptible" individuals) could experience irreversible or other serious, long-lasting effects or impaired ability to escape.

- AEGL-3: The airborne concentration of a substance at or above which it is predicted that the general population (including "susceptible" but excluding "hyper-susceptible" individuals) could experience life-threatening effects or death.

The AEGL-1 values are protective of sensitive subpopulations and are derived using methods that have a high degree of review. Most values are currently in draft form.

The NRC/COT states that the EEGL is a peak level of exposure and should not be considered as "hygienic" or "safe" (reference 11). The EEGLs were developed for rare emergency conditions and, therefore, represent levels that may cause more substantial effects than the primary levels cited by the preceding sources. This level of protection is equivalent to that of ERPG-2 and AEGL-2.

The IDLH values are published by the National Institute for Occupational Safety and Health (NIOSH). These represent 30-minute values that allow for a worker to escape injury or irreversible harm in the event of respiratory protection equipment failure (reference 10). These values were revised in 1994. Not all of these values were revised based on new toxicity information. In the 1994 revision, NIOSH made an *a priori* determination not to publish values higher than the existing values. The IDLH values are often equivalent to ERPG-3 and AEGL-3 values.

ACGIH has developed Short Term Exposure Levels (STELs) for substances that are irritating and are acutely toxic. The STEL is defined as a 15 minute time weighted average concentration to which it is believed that workers can be exposed continuously for a short period of time without suffering from 1) irritation, 2) chronic or irreversible tissue damage, or 3) narcosis of sufficient degree to increase the likelihood of accidental injury, impair self-rescue, or materially reduce work efficiency (reference 1).

2.0 Long-term Toxicity Benchmarks:
These values apply to exposures applicable to long term (subchronic or chronic) exposures. Several jurisdictions provide values consistent with this criterion, most intended to apply to occupational scenarios.

The NRC/COT has developed values for deployed military personnel for continuous exposures/deployments lasting up to 90 days (e.g., as in a submarine). In contrast to EEGLs, Continuous Exposure Guidance Levels (CEGLs) are not for use during emergencies but rather are intended to provide guidance for persistent exposures that should not cause serious or permanent effects (reference 11).

RfDs and RfCs are based on the assumption that thresholds exist for certain toxic effects such as cellular necrosis. The RfDs are expressed in units of mg/kg-day. In general, the RfD and RfC are estimates (with uncertainty spanning perhaps an order of magnitude) of a daily exposure to the human population (including sensitive subgroups) that is likely to be without an appreciable risk of deleterious effects during a lifetime (reference 2).

ATSDR has developed acute MRLs that are appropriate for continuous exposures from 1 to 14 days (reference 7). However, MRLs are derived using the no-observed adverse effect level (NOAEL) concentration and applying uncertainty factors (UFs) to extrapolate to the general population (including sensitive sub-populations but not hypersensitive individuals). The methodology used is consistent with that used by the EPA in the development of RfDs. Since these values are based on a NOAEL, adverse effects may not occur as a result of exposures to concentrations that slightly exceed the MRL. Carcinogenic endpoints were not considered in the development of MRLs .

ACGIH has published TLVs that are effect based and consider the typical working population exposed 8 hrs/day, 5 days/week, 50 weeks/year for 30 years (reference 1). ACGIH cautions against any other use. These TLVs are developed by the ACGIH Committee and are reviewed annually. Epidemiological data, as well as toxicological and toxicokinetic data, are used in the derivation of TLVs. Since occupational exposures can be chronic (i.e. exceeding 7 years), cancer is considered as an endpoint. Also considered is the 2/3 - (16-hour) daily break in exposure that may be important in the disposition of substances to which one is exposed in the workplace.

The EPA publishes MCLs to be used in assessing risk from chemicals in drinking water (reference 3). They have been developed for the general population and are often derived considering the limits of reliably detecting specific concentrations of substances in water. The MCL G (goals) are values that may not be achievable, but are goals based on toxicology information from which there is a toxicological basis. They are considered as "goals" since they are not regulation, and labeled as such since available detection or remediation technology precludes a lower value.

Similar to TLVs are Permissible Exposure Limits (PELs). The PELs are promulgated values developed by the Occupational Safety and Health Administration (OSHA). These values are time-weighted averages that below, which are acceptable for workplace scenarios (reference 9).

NIOSH has developed recommended exposure limits (RELs) for workplace exposures (reference 9). The NIOSH RELs are based on risk evaluations using human or animal health effects data, and on an assessment of what levels can be feasibly achieved by engineering controls and measured by analytical techniques. To the extent feasible, NIOSH RELs will project not only a no-effect exposure, but also exposure levels at which there may be residual risks.

APPENDIX C:

TABLE OF TOXICITY BENCHMARK VALUES

Firing Range Compounds of Suspected Concern									
		Ing. RfDo		**CSFo**		**Inh. RfDi**		**CSFi**	
Substance	**CAS**	mg/kg/d	**Ref**	1/mg/kg/d	**Ref**	mg/kg/d	**Ref**	1/mg/kg/d	**Ref**
(1,2-dichloroethyl)-benzene	1074-11-9								
1,2,4-Trimethylbenzene	95-63-6	5.00E-02	EPA-NCEA			1.70E-03	EPA-NCEA		
1,2-Dichlorethane	107-06-2	1.00E-001	HEAST	9.10E-02	IRIS	1.40E-01	A	7.40E-03	IRIS
1,2-Dichloro-3-methylbenzene	32768-54-0								
1,2-Dichloroethene	540-59-0 CIS	1.00E-02	HEAST						
1,2-Dichloroethene	TRANS	2.00E-02	IRIS						
1,3,5-Trimethylbenzene	108-67-8	5.00E-02	EPA-NCEA			1.70E-03	EPA-NCEA		
1,3,5-Trinitrobenzene	99-35-4	3.00E-02	IRIS						
1,3-Butadiene	106-99-0							0.08	IRIS
1,3-Dinitrobenzene	99-65-0	1.00E-04	IRIS						
1,4-Diamin-2,3-dihyroanthroquinone	81-63-0								
1,4-Di-p-toluidinoanthroquinone	128-80-3								
1-Butanol	71-36-3	1.00E-01	IRIS						
1-Butene	106-98-9								
1-Butene/Isobutylene									
1-Chloro-2-methylbenzene	95-49-8	2.00E-02	IRIS						
1-Chloro-3-methylbenzene	108-41-8								
1-Hexene	592-41-6								
1-Methylaminoanthraquinone	82-38-2								
1-Pentene	109-67-1								
2-(2-quinolinyl)-(H-indene-1,3-(2H)-dione (a)	83-08-9								
2-(2-quinolinyl)-1,3-indandione	8003-22-3								
2,3,7,8-Tetracholorodibenzo-p-dioxin	1746-01-6			1.50E+05	HEAST			1.50E+05	HEAST
2,3-Butanedione	431-03-8								
2,4,6-Trinitrotoluene	118-96-7	5.00E-04	IRIS	3.00E-02	IRIS				
2,4-Dinitrotoluene	121-14-2	2.00E-03	IRIS						
2,6-Dinitrotoluene	606-20-2	1.00E-03	HEAST						
2.5-Dimethylfuran	625-86-5								
2-Amino-4,6-Dinitrotoluene	35572-78-2	6.00E-05	EPA-NCEA						
2-amino-9,10-anthracenedione (a)	117-79-3								
2-Butanone	78-93-3	6.00E-01	IRIS			2.86E-01	IRIS		
2-Furaldehyde	98-01-1	3.00E-03	IRIS			1.00E-02	A		
2-Heptanone	110-43-0								
2-Methyl-1-butene	563-46-2								
2-Methylfuran	534-22-5								
2-Methylthiophene	554-14-3								
2-Nitrotoluene	88-72-2	1.00E-02	HEAST						
2-Pentanone	107-87-9								

Firing Range Compounds of Suspected Concern									
		Ing. RfDo		**CSFo**		**Inh. RfDi**		**CSFi**	
Substance	**CAS**	mg/kg/d	**Ref**	1/mg/kg/d	**Ref**	mg/kg/d	**Ref**	1/mg/kg/d	**Ref**
2-Propanol	67-63-0								
2-Thiophenecarboxaldehyde	98-03-3								
3-(phenylhydrazone)-1H-Indole-2,3-dione									
3-Furaldehyde	498-60-2								
3-Methyl-1-butene	563-45-1								
3-Methylfuran	930-27-8								
3-Methylthiophene	616-44-4								
3-Nitrotoluene	99-08-1	1.00E-02	EPA-NCEA						
4-1,2,4-oxadizaolin-3-one-2,5-diphenyl-delta									
4-Amino-2,6-Dinitrotoluene	19406-51-0								
4-Ethyltoluene	622-96-8								
4-Methyl-2-Pentanone	108-10-1	8.00E-02	HEAST			2.00E-02	A		
4-Nitrotoluene	99-99-0	1.00E-02	HEAST						
4-phenoxy-2(1H)-quinolinone (a)									
Acenaphthene	83-32-9	6.00E-02	IRIS						
Acenaphthylene	208-96-8								
Acetaldehyde	75-07-0					2.57E-03	IRIS	6.29E-04	IRIS
Acetic Acid	64-19-7								
Acetone	67-64-1	1.00E-01	IRIS						
Acetonitrile	75-05-8					1.7×10^{-2}	IRIS		
Acetophenone	98-86-2	1.00E-01	IRIS			5.70E-06	IRIS (WD)		
Acetylene	74-86-2								
Acrolein	107-02-8	2.00E-02	HEAST			5.7×10^{-6}	IRIS		
Acrylonitrile	107-13-1	3.00E-02	IRIS	5.40E-01	IRIS	5.7×10^{-4}	IRIS	1.94E-02	IRIS
Aluminum	7429-90-5	1.00E+00	EPA-NCEA			1.00E-03	EPA-NCEA		
Anthracene	120-12-7	3.00E-01	IRIS						
Antimony	7440-36-0	4.00E-04	IRIS						
Arsenic	7440-38-2	3.00E-04	IRIS	1.43E-03	IRIS			1.23E+00	IRIS
Barium	7440-39-3	7.00E-02	IRIS			1.40E-04	A		
Benzaldehyde	100-52-7	1.00E-01	IRIS						
Benzanthrone (b)	82-05-3								
Benzene	71-43-2	3.00E-03	EPA-NCEA	5.50E-02	IRIS	1.70E-03	EPA-NCEA	6.29E-04	IRIS
Benzo(a)anthracene	56-55-3			7.30E-01	EPA-NCEA			3.10E-01	EPA-NCEA
Benzo(a)pyrene	50-32-8			7.30E+00	IRIS			3.10E+00	EPA-NCEA
Benzo(b)fluoranthene	205-99-2			7.30E-01	EPA-NCEA			3.10E-01	EPA-NCEA
Benzo(e)pyrene	192-97-2								
Benzo(g,h,i)perylene	191-24-2								
Benzo(k)fluoranthene	207-08-9			7.30E-02	EPA-NCEA			3.10E-02	EPA-NCEA
Benzofuran	271-89-6								

Firing Range Compounds of Suspected Concern									
		Ing. RfDo		**CSFo**		**Inh. RfDi**		**CSFi**	
Substance	**CAS**	mg/kg/d	**Ref**	1/mg/kg/d	**Ref**	mg/kg/d	**Ref**	1/mg/kg/d	**Ref**
Benzonitrile	100-47-0								
Beryllium	7440-41-7	2.00E-03	IRIS			5.70E-06	IRIS	0.69	IRIS
Bis(2-ethylhexyl)phthalate	117-81-7	2.00E-02	IRIS	1.40E-02	IRIS			1.40E-02	EPA-NCEA
Butanal	123-72-8								
Cadmium	7440-43-9	1.00E-03	IRIS			5.70E-05	EPA-NCEA	0.51	IRIS
Calcium									
Carbon Dioxide (CO_2)	124-38-9								
Carbon Disulfide	75-15-0	1.00E-01	IRIS			2.00E-01	IRIS		
Carbon Monoxide (CO)	630-08-0								
Carbontetrachloride	56-23-5	7.00E-04	IRIS	1.06E-04	IRIS	5.71E-04	EPA-NCEA	4.29E-03	IRIS
Carbonyl Sulfide	463-58-1								
Chlorobenzene	108-90-7	2.00E-02	IRIS			1.70E-02	EPA-NCEA		
Chloroethene (vinyl chloride)	75-01-4	3.00E-03	IRIS	1.50E+00	IRIS	2.80E-02	IRIS	1.26E-03	IRIS
Chloroform	67-66-3	1.00E-02	IRIS	6.10E-03	IRIS	8.60E-05	EPA-NCEA	6.57E-03	IRIS
Chloromethane	74-87-3			7.30E-03	HEAST	8.60E-02	EPA-NCEA	3.50E-03	EPA-NCEA
Chromium	7440-47-3	3.00E-03	IRIS			3.00E-05	IRIS	2.90E+02	IRIS
Chrysene	218-01-9			7.30E-03	EPA-NCEA			3.10E-03	EPA-NCEA
cis-2-Butene	590-18-1								
Cl_2 (a)	7782-50-5	1.00E-01	IRIS			5.70E-05	EPA-NCEA		
Cobalt	7440-48-4	2.00E-02	EPA-NCEA			5.00E-06	EPA-NCEA		
Copper	7440-50-8	4.00E-02	HEAST						
Dibenz(a,h)anthracene	53-70-3								
Dibenzo(b,def)chrysene-7,14 dione									
Dibutyl phthalate	84-74-2	1.00E-01	IRIS						
Dichloroacetonitrile	3018-12-0								
Dichlorodiflouromethane	75-71-8	2.00E-01	IRIS			5.00E-02	A		
Dimethyltrisulfide	3658-80-8								
Dioctyl phthalate	117-81-7	2.00E-02	IRIS	1.40E-02	IRIS				
Dioxin TEQ (c)	19408-74-3			6.20E-03	IRIS			3.70E+02	IRIS
Diphenylamine	122-39-4	2.50E-02	IRIS						
Ethane	74-84-0								
Ethanol	64-17-5								
Ethylbenzene	100-41-4	1.00E-01	IRIS			2.90E-01	IRIS		
Ethylchloride	75-00-3					2.86E+00	IRIS		
Ethylene	74-85-1								
Fluoranthene	206-44-0								
Fluorene	86-73-7	4.00E-02	IRIS						
Formaldehyde	50-00-0	2.00E-01	IRIS					3.70E-04	IRIS

Firing Range Compounds of Suspected Concern									
		Ing. RfDo		**CSFo**		**Inh. RfDi**		**CSFi**	
Substance	**CAS**	mg/kg/d	**Ref**	1/mg/kg/d	**Ref**	mg/kg/d	**Ref**	1/mg/kg/d	**Ref**
Furan	110-00-9	1.00E-03	IRIS						
HCl	7647-01-0					5.70E-03	IRIS		
Heptanal	111-71-7								
Hexachlorobenzene	118-74-1	8.00E-04	IRIS	1.60E+00	IRIS			1.30E-01	IRIS
Hexachlorobutadiene	87-68-3	2.00E-04	HEAST	7.80E-02	IRIS			6.29E-03	IRIS
Hexachlorocyclopentadiene	77-47-4	6.00E-03	IRIS			2.00E-04	IRIS		
Hexachloroethane	67-72-1	1.00E-03	IRIS	1.40E-02	IRIS			1.14E-03	IRIS
Hexanal	66-25-1								
Hexane	110-54-3					5.71E-02	IRIS		
HMX	2691-41-0	5.00E-02	IRIS						
Hydrogen Cyanide	74-90-8	2.00E-02	IRIS			8.57E-04	IRIS		
i-Butane									
i-Butene									
Indeno(1,2,3-cd)pyrene									
Isothiocyanatomethane	556-61-6								
Lead	7439-92-1								
Magnesium	7439-95-4								
Manganese	7439-96-5	1.40E-01	IRIS			1.43E-05	IRIS		
m-Dichlorobenzene	541-73-1	9.00E-04	EPA-NCEA						
Mercury	7439-97-6					8.60E-05	IRIS		
Methacrolein	78-85-3								
Methane	74-82-8								
Methylene Chloride	75-09-2	6.00E-02	IRIS	7.50E-03	IRIS	8.60E-01	HEAST	1.34E+00	IRIS
Methylnitrite	624-91-9								
Methyl-t-butylether (MTBE)	1634-04-4					8.57E-01	IRIS		
Methyl-vinyl ketone	78-94-4								
m-Xylene	108-38-3	2.00E+00	IRIS						
Naphthalene	91-20-3	2.00E-02	IRIS			8.57E-04	IRIS		
n-Butane	106-97-8								
n-Decane	124-18-5								
NH3	7664-41-7					2.86E-02	IRIS		
n-Hexane	110-54-3	6.00E-02	HEAST			5.71E-02	IRIS		
Nickel	7440-02-0	2.00E-02				(2.00E-03)	ATSDR		
Nitric Acid	7697-37-2								
Nitrobenzene	98-95-3	5.00E-04	IRIS			6.00E-04	A		
Nitrogen Oxide (NOx)	10024-97-2	1.00E+00	IRIS (w)						
Nitroglycerine	55-63-0								
Nitromethane	75-52-5								
Nonanal									

Firing Range Compounds of Suspected Concern									
		Ing. RfDo		**CSFo**		**Inh. RfDi**		**CSFi**	
Substance	**CAS**	mg/kg/d	**Ref**	1/mg/kg/d	**Ref**	mg/kg/d	**Ref**	1/mg/kg/d	**Ref**
OCDD									
Octanal	124-13-0								
o-Dichlorobenzene	95-50-1	9.00E-02	IRIS						
o-methoxy-phenyl-azo-b-naphthol									
o-Xylene	95-47-6	2.00E+00	IRIS						
Particulate Cyanide	57-12-5	2.00E-02	IRIS						
p-Dichlorobenzene	106-46-7	3.00E-02	EPA-NCEA	2.40E-02	HEAST	2.29E-01	IRIS	2.20E-02	EPA-NCEA
Pentaerythritoltetranitrate									
Perchloroethylene	127-18-4	1.00E-02	IRIS	5.20E-02	EPA-NCEA	1.40E-01	EPA-NCEA	2.00E-03	EPA-NCEA
Phenanthrene	85-01-8								
Phenol	108-95-2	6.00E-01	IRIS						
Phenylacetylene	536-74-3								
Phosphorus	7723-14-0	2.00E-05	IRIS						
Propanal	123-38-6								
Propane	74-98-6								
Propene	115-07-1								
Propylene	115-07-1								
Propyne	74-99-7								
p-Xylene	106-42-3	2.00E+00	IRIS						
Pyrene	129-00-0	3.00E-02							
RDX	121-82-4	3.00E-03	IRIS	1.10E-01	IRIS				
Selenium	7782-49-2	5.00E-03	IRIS						
Silver	7440-22-4	5.00E-03	IRIS						
Styrene	100-42-5	2.00E-01	IRIS			2.86E-01	IRIS		
Sulfur Dioxide (SO2)	7446-09-5								
Sulfuric Acid	64-67-5								
Tetrachloroethene	127-18-4	1.00E-02	IRIS	5.20E-02	EPA-NCEA	1.40E-01	EPA-NCEA	2.00E-03	EPA-NCEA
Tetryl	479-45-8	1.00E-02	HEAST						
Thallium									
Thiophene	110-02-1								
Toluene	108-88-3	2.00E-01	IRIS			1.14E-01	IRIS		
trans-2-Butenal	123-73-9			1.90E+00	HEAST				
trans-2-Butene	624-64-6								
trans-2-Pentene	646-04-8								
trans-3-Penten-2-one	3102-33-8								
Trichloroethylene	79-01-6	6.00E-03	EPA-NCEA	1.10E-02	EPA-NCEA			6.00E-03	EPA-NCEA
Trichloroflouromethane	75-69-4	3.00E-01	IRIS			2.00E-01	A		
Vinylidenechloride									

Firing Range Compounds of Suspected Concern									
		Ing. RfDo		**CSFo**		**Inh. RfDi**		**CSFi**	
Substance	**CAS**	mg/kg/d	**Ref**	1/mg/kg/d	**Ref**	mg/kg/d	**Ref**	1/mg/kg/d	**Ref**
Zinc	7440-66-6	3.00E-01	IRIS						
a - Acute value									
l - Intermediate (subchronic) value									
c - Chronic value									

Firing Range Compounds of Suspected Concern			**MRLs**						
	TLV/TWA	**STEL**	**MRLs Inhalation**		**MRLs Oral**		**ERPG-1**	**ERPG-2**	**ERPG-3**
Substance	**ppm (mg/m3)**	**ppm (mg/m3)**	**ppm (mg/m3)**	duration	**mg/kg/day**	duration	ppm (mg/m3)	ppm (mg/m3)	ppm (mg/m3)
(1,2-dichloroethyl)-benzene									
1,2,4-Trimethylbenzene	1.00E+01								
1,2-Dichlorethane			6.00E-01	c	2.00E-01	i			
1,2-Dichloro-3-methylbenzene									
1,2-Dichloroethene					1.0 / 0.3	a/i			
1,2-Dichloroethene			0.2/0.2	a/i	2.00E-01	i			
1,3,5-Trimethylbenzene									
1,3,5-Trinitrobenzene									
1,3-Butadiene	2.00E+00						1.00E+01	2.00E+02	5.00E+02
1,3-Dinitrobenzene	1.50E-01				0.008 / 0.0005	a/i			
1,4-Diamin-2,3-dihyroanthroquinone									
1,4-Di-p-toluidinoanthroquinone									
1-Butanol		5.00E+01							
1-Butene									
1-Butene/Isobutylene									
1-Chloro-2-methylbenzene									
1-Chloro-3-methylbenzene									
1-Hexene	3.00E+01								
1-Methylaminoanthraquinone									
1-Pentene									
2-(2-quinolinyl)-(H-indene-1,3-(2H)-dione (a)									
2-(2-quinolinyl)-1,3-indandione									
2,3,7,8-Tetracholorodibenzo-p-dioxin					2E-7/2E-8/1E-9	a/i/c			
2,3-Butanedione									
2,4,6-Trinitrotoluene	(1.00E-01)				5.00E-04	i			
2,4-Dinitrotoluene	(2E-01)*				0.05/0.002	a/c			
2,6-Dinitrotoluene	(2E-01)*				4.00E-03	i			
2.5-Dimethylfuran									
2-Amino-4,6-Dinitrotoluene									
2-amino-9,10-anthracenedione (a)									
2-Butanone									
2-Furaldehyde									
2-Heptanone	5.00E+01								
2-Methyl-1-butene									
2-Methylfuran									
2-Methylthiophene									
2-Nitrotoluene	2.00E+00								

Firing Range Compounds of Suspected Concern			**MRLs**						
	TLV/TWA	**STEL**	**MRLs Inhalation**		**MRLs Oral**		**ERPG-1**	**ERPG-2**	**ERPG-3**
Substance	**ppm (mg/m3)**	**ppm (mg/m3)**	**ppm (mg/m3)**	duration	**mg/kg/day**	duration	ppm (mg/m3)	ppm (mg/m3)	ppm (mg/m3)
2-Pentanone									
2-Propanol									
2-Thiophenecarboxaldehyde									
3-(phenylhydrazone)-1H-Indole-2,3-dione									
3-Furaldehyde									
3-Methyl-1-butene									
3-Methylfuran									
3-Methylthiophene									
3-Nitrotoluene	2.00E+00								
4-1,2,4-oxadizaolin-3-one-2,5-diphenyl-delta									
4-Amino-2,6-Dinitrotoluene									
4-Ethyltoluene									
4-Methyl-2-Pentanone									
4-Nitrotoluene	2.00E+00								
4-phenoxy-2(1H)-quinolinone (a)									
Acenaphthene					6.00E-01	i			
Acenaphthylene									
Acetaldehyde		2.50E+01					1.00E+01	2.00E+02	1.00E+03
Acetic Acid	1.00E+01	1.50E+01							
Acetone	5.00E+02	7.50E+02	26/13/13	a/i/c	2.00E+00	i			
Acetonitrile	4.00E+01	6.00E+01							
Acetophenone	1.00E+01								
Acetylene									
Acrolein		1.00E-01	5E-5/ 9E-6	a/i	5.00E-04	a/c	1.00E-01	5.00E-01	3.00E+00
Acrylonitrile	2.00E+00		1.00E-01	a	0.1/.01/.04	a/i/c	1.00E+01	3.50E+01	7.50E+01
Aluminum	(1.00E+01)				2.00E+00	i			
Anthracene					1.00E+01	i			
Antimony	(5.00E-01)								
Arsenic	(1.00E-01)				0.005, 0.003	ac			
Barium	(5.00E-01)								
Benzaldehyde									
Benzanthrone (b)									
Benzene	(5.00E-01)	2.50E+00	0.05/0.004	a/i			5.00E+01	5.00E+01	1.00E+03
Benzo(a)anthracene									
Benzo(a)pyrene									
Benzo(b)fluoranthene									
Benzo(e)pyrene									
Benzo(g,h,i)perylene									
Benzo(k)fluoranthene									

Firing Range Compounds of Suspected Concern			**MRLs**						
	TLV/TWA	**STEL**	**MRLs Inhalation**		**MRLs Oral**		**ERPG-1**	**ERPG-2**	**ERPG-3**
Substance	**ppm (mg/m3)**	**ppm (mg/m3)**	**ppm (mg/m3)**	duration	**mg/kg/day**	duration	ppm (mg/m3)	ppm (mg/m3)	ppm (mg/m3)
Benzofuran									
Benzonitrile									
Beryllium	(2.00E-03)	(1.00E-02)			1.00E-03	c		(2.50E-01)	(1.00E-01)
Bis(2-ethylhexyl)phthalate	(5.00E+00)				0.01 (prov.)	i			
Butanal									
Cadmium	(1.00E-01)				2.00E-04	c			
Calcium									
Carbon Dioxide (CO_2)	(5.00E+03)	3.00E+04							
Carbon Disulfide	(1.00E+01)		3.00E-01	c	1.00E-02	a	1.00E+00	5.00E+01	5.00E+02
Carbon Monoxide (CO)	2.50E+01						2.00E+02	3.50E+02	5.00E+02
Carbontetrachloride	5.00E+00	1.00E+01	0.2/0.05	a/i	0.02/0.007	a/i	2.00E+01	1.00E+02	7.50E+02
Carbonyl Sulfide									
Chlorobenzene	1.00E+01				4.00E-01	i			
Chloroethene (vinyl chloride)	1.00E+00								
Chloroform	1.00E+01		0.1/0.05/0.02	a/i/c	0.3/0.1/0.01	a/i/c		5.00E+01	5.00E+03
Chloromethane	5.00E+01	1.00E+02	0.5/0.2/0.05	a/i/c				4.00E+02	1.00E+03
Chromium	(5.00E-01)								
Chrysene									
cis-2-Butene									
Cl_2 (a)								3.00E+00	2.00E+01
Cobalt	(2.00E-02)		(3.00E-05)	i					
Copper	(1.00E+00)								
Dibenz(a,h)anthracene									
Dibenzo(b,def)chrysene-7,14 dione									
Dibutyl phthalate	(5.00E+00)				3.00E+00	a			
Dichloroacetonitrile									
Dichlorodiflouromethane	1.00E+03								
Dimethyltrisulfide									
Dioctyl phthalate									
Dioxin TEQ (c)									
Diphenylamine	(1.00E+01)								
Ethane									
Ethanol									
Ethylbenzene	1.00E+02	1.25E+02	1.00E+00	i					
Ethylchloride	1.00E+02								
Ethylene									
Fluoranthene					4.00E-01	i			
Fluorene					4.00E-01	i			

Firing Range Compounds of Suspected Concern			**MRLs**						
	TLV/TWA	**STEL**	**MRLs Inhalation**		**MRLs Oral**		**ERPG-1**	**ERPG-2**	**ERPG-3**
Substance	**ppm (mg/m3)**	**ppm (mg/m3)**	**ppm (mg/m3)**	duration	**mg/kg/day**	duration	ppm (mg/m3)	ppm (mg/m3)	ppm (mg/m3)
Formaldehyde		3.00E-01	0.04/0.03/0.008	a/i/c	0.3/0.2	i/c	1.00E+00	1.00E+01	2.50E+01
Furan									
HCl		5.00E+00					3.00E+00	2.00E+01	1.50E+02
Heptanal									
Hexachlorobenzene	(2.00E-03)				8E-3/1E-4/2E-5	a/i/c			
Hexachlorobutadiene	2.00E-02				2.00E-04	i	3.00E+00	1.00E+01	3.00E+01
Hexachlorocyclopentadiene	1.00E-02		0.01/0.00002	i/c	1.00E-01	i			
Hexachloroethane	1.00E+00		6/6	a/i	1/0.01	a/i			
Hexanal									
Hexane									
HMX					0.1/0.05	ai			
Hydrogen Cyanide		4.70E+00						1.00E+01	2.50E+01
i-Butane									
i-Butene									
Indeno(1,2,3-cd)pyrene									
Isothiocyanatomethane									
Lead	(5.00E-02)								
Magnesium									
Manganese	(2.00E-01)		(4.00E-05)	c					
m-Dichlorobenzene									
Mercury	(2.50E-02)		(2.00E-04)	c					
Methacrolein									
Methane									
Methylene Chloride	5.00E+01		0.6/0.3/0.3	a/i/c	0.2/0.06	a/c	2.00E+02	7.50E+02	4.00E+03
Methylnitrite									
Methyl-t-butylether (MTBE)			2.0/ 0.7/ 0.7	a/i/c	0.4/0.3	a/i			
Methyl-vinyl ketone									
m-Xylene	1.00E+02	1.50E+02	6.00E-01	i					
Naphthalene	1.00E+01	1.50E+01	2.00E-03	c	0.05/0.02	a/i			
n-Butane									
n-Decane									
NH3	2.50E+01	3.50E+01	0.5/0.3	a/c	3.00E-01	i	2.50E+01	1.50E+02	7.50E+02
n-Hexane	5.00E+01		6.00E-01	c					
Nickel	(1.5E+00)		(2.00E-04)	c					
Nitric Acid	2.00E+00	4.00E+00					1.00E+00	6.00E+00	7.80E+01
Nitrobenzene	1.00E+00								
Nitrogen Oxide (NOx)	3.00E+00	5.00E+00							
Nitroglycerine									
Nitromethane	2.00E+01								

Firing Range Compounds of Suspected Concern			**MRLs**						
	TLV/TWA	**STEL**	**MRLs Inhalation**		**MRLs Oral**		**ERPG-1**	**ERPG-2**	**ERPG-3**
Substance	**ppm (mg/m3)**	**ppm (mg/m3)**	**ppm (mg/m3)**	duration	**mg/kg/day**	duration	ppm (mg/m3)	ppm (mg/m3)	ppm (mg/m3)
Nonanal									
OCDD									
Octanal									
o-Dichlorobenzene	2.50E+01								
o-methoxy-phenyl-azo-b-naphthol									
o-Xylene	1.00E+02		1/0.7/0.1	a/i/c	2.00E-01	i			
Particulate Cyanide									
p-Dichlorobenzene									
Pentaerythritoltetranitrate									
Perchloroethylene	2.50E+01	1.00E+02					1.00E+02	2.00E+02	1.00E+03
Phenanthrene									
Phenol	5.00E+00						1.00E+01	5.00E+01	2.00E+02
Phenylacetylene									
Phosphorus	2.00E-02		(2.00E-02)	a	2.00E-04	i			
Propanal									
Propane	2.50E+03								
Propene									
Propylene									
Propyne	1.00E+03								
p-Xylene	1.00E+02	1.50E+02	1.00E+00	a					
Pyrene									
RDX					0.06/0.03	a/i			
Selenium	(2.00E-01)				5.00E-03	c			
Silver	(1.00E-01)								
Styrene			6.00E-02	c	2.00E-01	i	5.00E+01	2.50E+02	1.00E+03
Sulfur Dioxide (SO2)	2.00E+00		1.00E-02	a			3.00E-01	3.00E+00	1.50E+01
Sulfuric Acid							(2.00E+00)	(1.00E+01)	(3.00E+01)
Tetrachloroethene									
Tetryl									
Thallium									
Thiophene									
Toluene			1/0.08	a/c	0.8/0.02	a/i	5.00E+01	3.00E+02	1.00E+03
trans-2-Butenal									
trans-2-Butene									
trans-2-Pentene									
trans-3-Penten-2-one									
Trichloroethylene	5.00E+01		2/0.1	a/i	2.00E-01	a	1.00E+02	5.00E+02	5.00E+03
Trichloroflouromethane									

Firing Range Compounds of Suspected Concern			**MRLs**						
	TLV/TWA	**STEL**	**MRLs Inhalation**		**MRLs Oral**		**ERPG-1**	**ERPG-2**	**ERPG-3**
Substance	**ppm (mg/m3)**	**ppm (mg/m3)**	**ppm (mg/m3)**	duration	**mg/kg/day**	duration	ppm (mg/m3)	ppm (mg/m3)	ppm (mg/m3)
Vinylidenechloride									
Zinc					0.3/0.3	i/c			
a - Acute value									
I - Intermediate (subchronic) value									
c - Chronic value									

Firing Range Compounds of Suspected Concern									
	AEGL-1	**ppm (mg/m3)**				**AEGL-2**	**ppm (mg/m3)**		
Substance	10 min	30 min	60 min	4 hr	8 hr	10 min	30 min	60 min	4 hr
(1,2-dichloroethyl)-benzene									
1,2,4-Trimethylbenzene									
1,2-Dichlorethane									
1,2-Dichloro-3-methylbenzene									
1,2-Dichloroethene									
1,2-Dichloroethene									
1,3,5-Trimethylbenzene									
1,3,5-Trinitrobenzene									
1,3-Butadiene									
1,3-Dinitrobenzene									
1,4-Diamin-2,3-dihyroanthroquinone									
1,4-Di-p-toluidinoanthroquinone									
1-Butanol									
1-Butene									
1-Butene/Isobutylene									
1-Chloro-2-methylbenzene									
1-Chloro-3-methylbenzene									
1-Hexene									
1-Methylaminoanthraquinone									
1-Pentene									
2-(2-quinolinyl)-(H-indene-1,3-(2H)-dione (a)									
2-(2-quinolinyl)-1,3-indandione									
2,3,7,8-Tetracholorodibenzo-p-dioxin									
2,3-Butanedione									
2,4,6-Trinitrotoluene									
2,4-Dinitrotoluene									
2,6-Dinitrotoluene									
2.5-Dimethylfuran									
2-Amino-4,6-Dinitrotoluene									
2-amino-9,10-anthracenedione (a)									
2-Butanone									
2-Furaldehyde									
2-Heptanone									
2-Methyl-1-butene									
2-Methylfuran									
2-Methylthiophene									

Firing Range Compounds of Suspected Concern									
	AEGL-1	**ppm (mg/m3)**				**AEGL-2**	**ppm (mg/m3)**		
Substance	10 min	30 min	60 min	4 hr	8 hr	10 min	30 min	60 min	4 hr
2-Nitrotoluene									
2-Pentanone									
2-Propanol									
2-Thiophenecarboxaldehyde									
3-(phenylhydrazone)-1H-Indole-2,3-dione									
3-Furaldehyde									
3-Methyl-1-butene									
3-Methylfuran									
3-Methylthiophene									
3-Nitrotoluene									
4-1,2,4-oxadizaolin-3-one-2,5-diphenyl-delta									
4-Amino-2,6-Dinitrotoluene									
4-Ethyltoluene									
4-Methyl-2-Pentanone									
4-Nitrotoluene									
4-phenoxy-2(1H)-quinolinone (a)									
Acenaphthene									
Acenaphthylene									
Acetaldehyde									
Acetic Acid									
Acetone									
Acetonitrile									
Acetophenone									
Acetylene									
Acrolein	3.00E-02	3.00E-02	3.00E-02	3.00E-02	3.00E-02	4.40E-01	1.80E-01	1.00E-01	1.00E-01
Acrylonitrile									
Aluminum									
Anthracene									
Antimony									
Arsenic									
Barium									
Benzaldehyde									
Benzanthrone (b)									
Benzene									
Benzo(a)anthracene									
Benzo(a)pyrene									
Benzo(b)fluoranthene									
Benzo(e)pyrene									
Benzo(g,h,i)perylene									

Firing Range Compounds of Suspected Concern									
	AEGL-1	**ppm (mg/m3)**				**AEGL-2**	**ppm (mg/m3)**		
Substance	10 min	30 min	60 min	4 hr	8 hr	10 min	30 min	60 min	4 hr
Benzo(k)fluoranthene									
Benzofuran									
Benzonitrile									
Beryllium									
Bis(2-ethylhexyl)phthalate									
Butanal									
Cadmium									
Calcium									
Carbon Dioxide (CO_2)									
Carbon Disulfide									
Carbon Monoxide (CO)									
Carbontetrachloride		1.60E+01	1.20E+01	6.90E+00	5.20E+00		9.00E+01	6.80E+01	3.90E+01
Carbonyl Sulfide									
Chlorobenzene									
Chloroethene (vinyl chloride)									
Chloroform							120	88	44
Chloromethane									
Chromium									
Chrysene									
cis-2-Butene									
Cl_2 (a)		1	1	0.5	0.5		3	2	1
Cobalt									
Copper									
Dibenz(a,h)anthracene									
Dibenzo(b,def)chrysene-7,14 dione									
Dibutyl phthalate									
Dichloroacetonitrile									
Dichlorodiflouromethane									
Dimethyltrisulfide									
Dioctyl phthalate									
Dioxin TEQ (c)									
Diphenylamine									
Ethane									
Ethanol									
Ethylbenzene									
Ethylchloride									
Ethylene									

Firing Range Compounds of Suspected Concern									
	AEGL-1	**ppm (mg/m3)**				**AEGL-2**	**ppm (mg/m3)**		
Substance	10 min	30 min	60 min	4 hr	8 hr	10 min	30 min	60 min	4 hr
Fluoranthene									
Fluorene									
Formaldehyde									
Furan	N/A	N/A	N/A	N/A	N/A	1.80E+01	1.30E+01	1.00E+01	2.50E+00
HCl	1.80E+00	1.80E+00	1.80E+00	1.80E+00	1.80E+00	1.00E+02	4.30E+01	2.20E+01	5.40E+00
Heptanal									
Hexachlorobenzene									
Hexachlorobutadiene									
Hexachlorocyclopentadiene									
Hexachloroethane									
Hexanal									
Hexane									
HMX									
Hydrogen Cyanide	2.50E+00	2.50E+00	2.00E+00	1.30E+00	1.00E+00	1.70E+01	1.00E+01	7.10E+00	3.50E+00
i-Butane									
i-Butene									
Indeno(1,2,3-cd)pyrene									
Isothiocyanatomethane									
Lead									
Magnesium									
Manganese									
m-Dichlorobenzene									
Mercury									
Methacrolein									
Methane									
Methylene Chloride									
Methylnitrite									
Methyl-t-butylether (MTBE)									
Methyl-vinyl ketone									
m-Xylene									
Naphthalene									
n-Butane									
n-Decane									
NH3	25(5min)	2.50E+01	2.50E+01	2.50E+01	2.50E+01	380(5min)	160	110	110
n-Hexane									
Nickel									
Nitric Acid		5.00E-01	5.00E-01	5.00E-01	5.00E-01		5.00E+00	4.00E+00	3.00E+00
Nitrobenzene									
Nitrogen Oxide (NOx)		5.00E-01	5.00E-01	5.00E-01	5.00E-01		1.50E+01	1.20E+01	8.20E+00

Firing Range Compounds of Suspected Concern									
	AEGL-1	**ppm (mg/m3)**				**AEGL-2**	**ppm (mg/m3)**		
Substance	10 min	30 min	60 min	4 hr	8 hr	10 min	30 min	60 min	4 hr
Nitroglycerine									
Nitromethane									
Nonanal									
OCDD									
Octanal									
o-Dichlorobenzene									
o-methoxy-phenyl-azo-b-naphthol									
o-Xylene									
Particulate Cyanide									
p-Dichlorobenzene									
Pentaerythritoltetranitrate									
Perchloroethylene									
Phenanthrene									
Phenol									
Phenylacetylene									
Phosphorus									
Propanal									
Propane									
Propene									
Propylene									
Propyne									
p-Xylene									
Pyrene									
RDX									
Selenium									
Silver									
Styrene									
Sulfur Dioxide (SO2)									
Sulfuric Acid									
Tetrachloroethene									
Tetryl									
Thallium									
Thiophene									
Toluene		1.20E+02	8.20E+01	4.10E+01	2.90E+01		2.70E+02	1.90E+02	9.40E+01
trans-2-Butenal									
trans-2-Butene									
trans-2-Pentene									

Firing Range Compounds of Suspected Concern									
	AEGL-1	**ppm (mg/m3)**				**AEGL-2**	**ppm (mg/m3)**		
Substance	10 min	30 min	60 min	4 hr	8 hr	10 min	30 min	60 min	4 hr
trans-3-Penten-2-one									
Trichloroethylene									
Trichloroflouromethane									
Vinylidenechloride									
Zinc									
a - Acute value									
l - Intermediate (subchronic) value									
c - Chronic value									

Firing Range Compounds of Suspected Concern										
		AEGL-3	**ppm (mg/m3)**				**CEGL**	**EEGL**	**EEGL**	**EEGL-1hr**
Substance	8 hr	10 min	30 min	60 min	4 hr	8 hr	ppm (mg/m3)	ppm (mg/m3)	ppm (mg/m3)	ppm (mg/m3)
(1,2-dichloroethyl)-benzene										
1,2,4-Trimethylbenzene										
1,2-Dichlorethane										
1,2-Dichloro-3-methylbenzene										
1,2-Dichloroethene										
1,2-Dichloroethene										
1,3,5-Trimethylbenzene										
1,3,5-Trinitrobenzene										
1,3-Butadiene										
1,3-Dinitrobenzene										
1,4-Diamin-2,3-dihyroanthroquinone										
1,4-Di-p-toluidinoanthroquinone										
1-Butanol										
1-Butene										
1-Butene/Isobutylene										
1-Chloro-2-methylbenzene										
1-Chloro-3-methylbenzene										
1-Hexene										
1-Methylaminoanthraquinone										
1-Pentene										
2-(2-quinolinyl)-(H-indene-1,3-(2H)-dione (a)										
2-(2-quinolinyl)-1,3-indandione										
2,3,7,8-Tetracholorodibenzo-p-dioxin										
2,3-Butanedione										
2,4,6-Trinitrotoluene										
2,4-Dinitrotoluene										
2,6-Dinitrotoluene										
2.5-Dimethylfuran										
2-Amino-4,6-Dinitrotoluene										
2-amino-9,10-anthracenedione (a)										
2-Butanone										
2-Furaldehyde										
2-Heptanone										
2-Methyl-1-butene										
2-Methylfuran										
2-Methylthiophene										
2-Nitrotoluene										

Firing Range Compounds of Suspected Concern										
		AEGL-3	**ppm (mg/m3)**				**CEGL**	**EEGL**	**EEGL**	**EEGL-1hr**
Substance	8 hr	10 min	30 min	60 min	4 hr	8 hr	ppm (mg/m3)	ppm (mg/m3)	ppm (mg/m3)	ppm (mg/m3)
2-Pentanone										
2-Propanol										
2-Thiophenecarboxaldehyde										
3-(phenylhydrazone)-1H-Indole-2,3-dione										
3-Furaldehyde										
3-Methyl-1-butene										
3-Methylfuran										
3-Methylthiophene										
3-Nitrotoluene										
4-1,2,4-oxadizaolin-3-one-2,5-diphenyl-delta										
4-Amino-2,6-Dinitrotoluene										
4-Ethyltoluene										
4-Methyl-2-Pentanone										
4-Nitrotoluene										
4-phenoxy-2(1H)-quinolinone (a)										
Acenaphthene										
Acenaphthylene										
Acetaldehyde										N/A
Acetic Acid										
Acetone							2.00E+02			8.50E+03
Acetonitrile										
Acetophenone										
Acetylene										
Acrolein	1.00E-01	6.20E+00	2.50E+00	1.40E+00	4.80E-01	2.70E-01	1.00E-02		0.1(10min)	5.00E-02
Acrylonitrile										
Aluminum										
Anthracene										
Antimony										
Arsenic										
Barium										
Benzaldehyde										
Benzanthrone (b)										
Benzene										5.00E+01
Benzo(a)anthracene										
Benzo(a)pyrene										
Benzo(b)fluoranthene										
Benzo(e)pyrene										
Benzo(g,h,i)perylene										
Benzo(k)fluoranthene										

Firing Range Compounds of Suspected Concern										
		AEGL-3	**ppm (mg/m3)**				**CEGL**	**EEGL**	**EEGL**	**EEGL-1hr**
Substance	8 hr	10 min	30 min	60 min	4 hr	8 hr	ppm (mg/m3)	ppm (mg/m3)	ppm (mg/m3)	ppm (mg/m3)
Benzofuran										
Benzonitrile										
Beryllium										
Bis(2-ethylhexyl)phthalate										
Butanal										
Cadmium										
Calcium										
Carbon Dioxide (CO_2)										
Carbon Disulfide								2000(10min)	100(30min)	5.00E+01
Carbon Monoxide (CO)							2.00E+01	1500(10min)	800(30min)	4.00E+02
Carbontetrachloride	3.00E+01		2.30E+02	1.70E+02	9.90E+01	7.50E+01				
Carbonyl Sulfide										
Chlorobenzene										
Chloroethene (vinyl chloride)										
Chloroform	31		9.20E+02	6.50E+02	3.30E+02	2.30E+02	1.00E+00			1.00E+02
Chloromethane										
Chromium										
Chrysene										
cis-2-Butene										
Cl_2 (a)	0.7		3.10E+01	2.20E+01	1.10E+01	8.00E+00	1.00E-01			3.00E+00
Cobalt										
Copper										
Dibenz(a,h)anthracene										
Dibenzo(b,def)chrysene-7,14 dione										
Dibutyl phthalate										
Dichloroacetonitrile										
Dichlorodiflouromethane							1.00E+02			1.00E+04
Dimethyltrisulfide										
Dioctyl phthalate										
Dioxin TEQ (c)										
Diphenylamine										
Ethane										
Ethanol										
Ethylbenzene										
Ethylchloride										
Ethylene										
Fluoranthene										
Fluorene										

Firing Range Compounds of Suspected Concern										
		AEGL-3	**ppm (mg/m3)**				**CEGL**	**EEGL**	**EEGL**	**EEGL-1hr**
Substance	8 hr	10 min	30 min	60 min	4 hr	8 hr	ppm (mg/m3)	ppm (mg/m3)	ppm (mg/m3)	ppm (mg/m3)
Formaldehyde										
Furan	1.30E+00	5.20E+01	4.60E+01	2.90E+01	7.10E+00	3.60E+00				
HCl	2.70E+00	6.20E+02	2.10E+02	1.04E+02	2.60E+01	1.30E+01	5.00E-01		100(10min)	2.00E+01
Heptanal										
Hexachlorobenzene										
Hexachlorobutadiene										
Hexachlorocyclopentadiene										
Hexachloroethane										
Hexanal										
Hexane										
HMX										
Hydrogen Cyanide	2.50E+00	2.70E+01	2.10E+01	1.50E+01	8.60E+00	6.60E+00				
i-Butane										
i-Butene										
Indeno(1,2,3-cd)pyrene										
Isothiocyanatomethane										
Lead										
Magnesium										
Manganese										
m-Dichlorobenzene										
Mercury							(0.01)			
Methacrolein										
Methane							5000			
Methylene Chloride										
Methylnitrite										
Methyl-t-butylether (MTBE)										
Methyl-vinyl ketone										
m-Xylene										2.00E+02
Naphthalene										
n-Butane										
n-Decane										
NH3	110	3800(5min)	1600	1100	550	390				1.00E+02
n-Hexane										
Nickel										
Nitric Acid	2.00E+00		2.70E+01	2.20E+01	1.50E+01	1.20E+01				
Nitrobenzene										
Nitrogen Oxide (NOx)	6.70E+00		2.50E+01	2.00E+01	1.40E+01	1.10E+01				
Nitroglycerine										
Nitromethane										

Firing Range Compounds of Suspected Concern										
		AEGL-3	**ppm (mg/m3)**				**CEGL**	**EEGL**	**EEGL**	**EEGL-1hr**
Substance	8 hr	10 min	30 min	60 min	4 hr	8 hr	ppm (mg/m3)	ppm (mg/m3)	ppm (mg/m3)	ppm (mg/m3)
Nonanal										
OCDD										
Octanal										
o-Dichlorobenzene										
o-methoxy-phenyl-azo-b-naphthol										
o-Xylene										2.00E+02
Particulate Cyanide										
p-Dichlorobenzene										
Pentaerythritoltetranitrate										
Perchloroethylene										
Phenanthrene										
Phenol										
Phenylacetylene										
Phosphorus										
Propanal										
Propane										
Propene										
Propylene										
Propyne										
p-Xylene										2.00E+02
Pyrene										
RDX										
Selenium										
Silver										
Styrene										
Sulfur Dioxide (SO2)							1.00E+00	(30,10min)	(20, 30min)	1.00E+01)
Sulfuric Acid								(5, 10min)	(2, 30min)	(1.00E+00)
Tetrachloroethene										
Tetryl										
Thallium										
Thiophene										
Toluene	6.70E+01		9.00E+02	6.30E+02	3.20E+02	2.20E+02	2.00E+01			2.00E+02
trans-2-Butenal										
trans-2-Butene										
trans-2-Pentene										
trans-3-Penten-2-one										
Trichloroethylene										2.00E+02
Trichloroflouromethane							1.00E+02			1.50E+03

Firing Range Compounds of Suspected Concern										
		AEGL-3	**ppm (mg/m3)**				**CEGL**	**EEGL**	**EEGL**	**EEGL-1hr**
Substance	8 hr	10 min	30 min	60 min	4 hr	8 hr	ppm (mg/m3)	ppm (mg/m3)	ppm (mg/m3)	ppm (mg/m3)
Vinylidenechloride							1.50E-01			
Zinc										
a - Acute value										
I - Intermediate (subchronic) value										
c - Chronic value										

Firing Range Compounds of Suspected Concern						
	EEGL-24hr	**MCLG**	**MCL**	**IDLH**	**PEL**	**REL**
Substance	ppm (mg/m3)	mg/L	mg/L	ppm (mg/m3)	ppm (mg/m3)	ppm (mg/m3)
(1,2-dichloroethyl)-benzene						
1,2,4-Trimethylbenzene						
1,2-Dichlorethane		0	5.00E-03			
1,2-Dichloro-3-methylbenzene						
1,2-Dichloroethene						
1,2-Dichloroethene						
1,3,5-Trimethylbenzene						
1,3,5-Trinitrobenzene						
1,3-Butadiene				2.00E+04	1.00E+03	N/A
1,3-Dinitrobenzene				(5.00E+01)	(1.00E+00)	(1.00E+00)
1,4-Diamin-2,3-dihyroanthroquinone						
1,4-Di-p-toluidinoanthroquinone						
1-Butanol						
1-Butene						
1-Butene/Isobutylene						
1-Chloro-2-methylbenzene						
1-Chloro-3-methylbenzene						
1-Hexene						
1-Methylaminoanthraquinone						
1-Pentene						
2-(2-quinolinyl)-(H-indene-1,3-(2H)-dione (a)						
2-(2-quinolinyl)-1,3-indandione						
2,3,7,8-Tetracholorodibenzo-p-dioxin		0	3.00E-08			
2,3-Butanedione						
2,4,6-Trinitrotoluene				5.00E+02	(1.50E+00)	(5.00E-01)
2,4-Dinitrotoluene				5.00E+01	(1.50E+00)	(1.50E+00)
2,6-Dinitrotoluene				5.00E+01	(1.50E+00)	(1.50E+00)
2.5-Dimethylfuran						
2-Amino-4,6-Dinitrotoluene						
2-amino-9,10-anthracenedione (a)						
2-Butanone						
2-Furaldehyde						
2-Heptanone				8.00E+02	1.00E+02	1.00E+02
2-Methyl-1-butene						
2-Methylfuran						
2-Methylthiophene						
2-Nitrotoluene				2.00E+02	5.00E+00	2.00E+00

Firing Range Compounds of Suspected Concern						
	EEGL-24hr	**MCLG**	**MCL**	**IDLH**	**PEL**	**REL**
Substance	ppm (mg/m3)	mg/L	mg/L	ppm (mg/m3)	ppm (mg/m3)	ppm (mg/m3)
2-Pentanone				1.50E+03	2.00E+02	1.50E+02
2-Propanol						
2-Thiophenecarboxaldehyde						
3-(phenylhydrazone)-1H-Indole-2,3-dione						
3-Furaldehyde						
3-Methyl-1-butene						
3-Methylfuran						
3-Methylthiophene						
3-Nitrotoluene				2.00E+02	5.00E+00	2.00E+00
4-1,2,4-oxadizaolin-3-one-2,5-diphenyl-delta						
4-Amino-2,6-Dinitrotoluene						
4-Ethyltoluene						
4-Methyl-2-Pentanone						
4-Nitrotoluene				2.00E+02	5.00E+00	2.00E+00
4-phenoxy-2(1H)-quinolinone (a)						
Acenaphthene						
Acenaphthylene						
Acetaldehyde	N/A			2.00E+03	2.00E+02	N/A
Acetic Acid				1.00E+03	1.00E+01	1.00E+01
Acetone	1.00E+03			2.00E+04	1.00E+03	2.50E+02
Acetonitrile				4.00E+03	4.00E+01	2.00E+01
Acetophenone						
Acetylene						
Acrolein	1.00E-02			5.00E+00	1.00E-01	1.00E-01
Acrylonitrile				5.00E+02	2.00E+00	1.00E+00
Aluminum						
Anthracene						
Antimony						
Arsenic		N/A	5.00E-02	(1.00E+02)	(1.00E-01)	(2.00E-03)
Barium				(1.10E+03)	(5.00E-01)	(5.00E-01)
Benzaldehyde						
Benzanthrone (b)						
Benzene	2.00E+00	0	5.00E-03	3.00E+03	1.00E+00	1.00E-01
Benzo(a)anthracene						
Benzo(a)pyrene		0	2.00E-04			
Benzo(b)fluoranthene						
Benzo(e)pyrene						
Benzo(g,h,i)perylene						
Benzo(k)fluoranthene						

Firing Range Compounds of Suspected Concern						
	EEGL-24hr	**MCLG**	**MCL**	**IDLH**	**PEL**	**REL**
Substance	ppm (mg/m3)	mg/L	mg/L	ppm (mg/m3)	ppm (mg/m3)	ppm (mg/m3)
Benzofuran						
Benzonitrile						
Beryllium		0.004	4.00E-03	(1.00E+00)	(2.00E-03)	(>5.00E-04)
Bis(2-ethylhexyl)phthalate		0	6.00E-03			
Butanal						
Cadmium		5.00E-03	5.00E-03	(5.00E+00)	(5.00E-03)	N/A
Calcium						
Carbon Dioxide (CO_2)				4.00E+04	5.00E+03	5.00E+03
Carbon Disulfide				5.00E+02	4.00E+00	1.00E+00
Carbon Monoxide (CO)	5.00E+01			1.50E+03	5.00E+01	3.50E+01
Carbontetrachloride		0.00E+00	5.00E-03	3.00E+02	1.00E+01	2.00E+00
Carbonyl Sulfide						
Chlorobenzene		1.00E-01	1.00E-01	2.40E+03	7.50E+01	N/A
Chloroethene (vinyl chloride)						
Chloroform	3.00E+01			1.00E+03	5.00E+01	2.00E+00
Chloromethane				2.00E+03	1.00E+02	
Chromium		1.00E-01	(1.00E-01)	(2.50E+01)		
Chrysene						
cis-2-Butene						
Cl_2 (a)	5.00E-01	4.00E+00	4.00E+00	3.00E+01	1.00E+00	5.00E-01
Cobalt						
Copper		1.30E+00	1.30E+00	(2.00E+03)	(1.00E+00)	(1.00E+00)
Dibenz(a,h)anthracene						
Dibenzo(b,def)chrysene-7,14 dione						
Dibutyl phthalate				(9.30E+03)	(5.00E+00)	(5.00E+00)
Dichloroacetonitrile						
Dichlorodiflouromethane	1.00E+03			5.00E+04	1.00E+03	1.00E+03
Dimethyltrisulfide						
Dioctyl phthalate						
Dioxin TEQ (c)						
Diphenylamine						
Ethane						
Ethanol				1.50E+04	1.00E+03	1.00E+03
Ethylbenzene		7.00E-01	7.00E-01	2.00E+03	1.00E+02	1.00E+02
Ethylchloride				2.00E+04	1.00E+03	N/A
Ethylene						
Fluoranthene						
Fluorene						

Firing Range Compounds of Suspected Concern						
	EEGL-24hr	**MCLG**	**MCL**	**IDLH**	**PEL**	**REL**
Substance	ppm (mg/m3)	mg/L	mg/L	ppm (mg/m3)	ppm (mg/m3)	ppm (mg/m3)
Formaldehyde				3.00E+01	7.50E-01	1.60E-02
Furan				2.50E+02	5.00E+00	
HCl	2.00E+01			1.00E+02	5.00E+00	5.00E+00
Heptanal						
Hexachlorobenzene		0.00E+00	1.00E-03			
Hexachlorobutadiene						
Hexachlorocyclopentadiene		5.00E-02	5.00E-02			
Hexachloroethane				3.00E+02	1.00E+00	1.00E+00
Hexanal						
Hexane						
HMX						
Hydrogen Cyanide				5.00E+01	1.00E+01	4.70E+00
i-Butane						
i-Butene						
Indeno(1,2,3-cd)pyrene						
Isothiocyanatomethane						
Lead		0.00E+00	1.50E-02			
Magnesium						
Manganese				(1.00E+04)	(5.00E+00)	(1.00E+00)
m-Dichlorobenzene						
Mercury	(2.00E-02)	2.00E-03	2.00E-03	(2.80E+01)	(1.00E-01)	(5.00E-02)
Methacrolein						
Methane	5.00E+03					
Methylene Chloride				5.00E+03	5.00E+02	N/A
Methylnitrite						
Methyl-t-butylether (MTBE)						
Methyl-vinyl ketone						
m-Xylene	1.00E+02	1.00E+01	1.00E+01	1.00E+03	1.00E+02	1.00E+02
Naphthalene				5.00E+02	1.00E+01	1.00E+01
n-Butane						
n-Decane						
NH3	1.00E+02			5.00E+02	5.00E+01	2.50E+01
n-Hexane				5.00E+03	5.00E+02	5.00E+01
Nickel				(2.00E+03)	(1.00E+00)	(1.50E-02)
Nitric Acid				1.00E+02	2.00E+00	2.00E+00
Nitrobenzene				2.00E+02	1.00E+00	1.00E+00
Nitrogen Oxide (NOx)				2.00E+01	5.00E+00	1.00E+00
Nitroglycerine				(5.00E+02)	(2.00E+00)	(1.00E-01)
Nitromethane				1.00E+03	1.00E+02	N/A

Firing Range Compounds of Suspected Concern						
	EEGL-24hr	**MCLG**	**MCL**	**IDLH**	**PEL**	**REL**
Substance	ppm (mg/m3)	mg/L	mg/L	ppm (mg/m3)	ppm (mg/m3)	ppm (mg/m3)
Nonanal						
OCDD						
Octanal						
o-Dichlorobenzene						
o-methoxy-phenyl-azo-b-naphthol						
o-Xylene	1.00E+02	1.00E+01	1.00E+01	1.00E+03	1.00E+02	1.00E+02
Particulate Cyanide						
p-Dichlorobenzene						
Pentaerythritoltetranitrate						
Perchloroethylene						
Phenanthrene						
Phenol				2.50E+02	5.00E+00	5.00E+00
Phenylacetylene						
Phosphorus				(2.00E+02)	(1.00E-01)	(1.00E-01)
Propanal						
Propane				2.00E+04	1.00E+03	1.00E+03
Propene						
Propylene						
Propyne						
p-Xylene	1.00E+02	1.00E+01	1.00E+01	1.00E+03	1.00E+02	1.00E+02
Pyrene						
RDX						
Selenium		5.00E-02	5.00E-02	(1.00E+02)	(2.00E-01)	(2.00E-01)
Silver				(2.00E+01)	(1.00E-02)	(1.00E-02)
Styrene		1.00E-01	1.00E-01	5.00E+03	1.00E+02	5.00E+01
Sulfur Dioxide (SO2)	5.00E+00			1.00E+02	5.00E+00	2.00E+00
Sulfuric Acid				(8.00E+01)	(1.00E+00)	(1.00E+00)
Tetrachloroethene						
Tetryl				(3.00E+03)	(1.50E+00)	(1.50E+00)
Thallium		5.00E-04	5.00E-04	(2.00E+01)	(1.00E-01)	(1.00E-01)
Thiophene						
Toluene	1.00E+02	1.00E+00	1.00E+00	2.00E+03	2.00E+02	1.00E+02
trans-2-Butenal						
trans-2-Butene						
trans-2-Pentene						
trans-3-Penten-2-one						
Trichloroethylene	1.00E+01	0.00E+00	5.00E-03	1.00E+03	1.00E+02	2.00E+00
Trichloroflouromethane	5.00E+02					

Firing Range Compounds of Suspected Concern						
	EEGL-24hr	**MCLG**	**MCL**	**IDLH**	**PEL**	**REL**
Substance	ppm (mg/m3)	mg/L	mg/L	ppm (mg/m3)	ppm (mg/m3)	ppm (mg/m3)
Vinylidenechloride	1.00E+01					
Zinc						
a - Acute value						
I - Intermediate (subchronic) value						
c - Chronic value						

Appendix C
Glossary of Physicochemical Properties

This appendix provides definitions of the properties and their units.

Physical and Chemical Properties

Parameters in this group describe basic physical properties for the constituent.

Contaminant name: Text descriptions of the constituent name to better identify chemicals.

CAS Registry Number: A unique accession number assigned by the Chemical Abstracts Service (http://www.cas.org/), a division of the American Chemical Society (http://www.acs.org/portal/Chemistry). CAS Registry Numbers are assigned to every uniquely identifiable substance, so "cis-2-hexene," "trans-2-hexene," and "2-hexene" (a mixture with unspecified cis/trans composition) are all assigned separate CAS Numbers.

Molecular weight: The molecular weight of a compound is measured in g/mole. Generally, the higher the molecular weight, the less soluble in water. Molecular weight also affects the density of a compound.

Molecular formula: The molecular formula of a compound showing the number of atoms of each type in the molecule.

Water solubility: Solubility is the measurement of the maximum concentration of a chemical that will dissolve in pure water at a specific temperature, measured in mg/L. Water solubility plays a large role in movement and distribution of a chemical through soil and groundwater.

Water solubility temperature: The water solubility temperature is the temperature corresponding to the water solubility value. For consistency with other parameters in the database, water solubility is usually defined at 25 ºC.

Vapor pressure: The vapor pressure of a chemical is the pressure exerted by its vapor, at a given temperature, in equilibrium with the pure compound (liquid or solid). Vapor pressure represents the tendency of a compound to evaporate. High vapor pressures mean that the compound is more likely to volatilize out of solution (mm Hg).

Vapor pressure temperature: The vapor pressure temperature is the temperature corresponding to the vapor pressure value. For consistency with other parameters in the database, vapor pressure is usually defined at 25 ºC.

Partitioning Factors

Parameters used to evaluate the distribution between media in the environment are included in this group.

Henry's law constant: The Henry's Law constant is a property of a chemical that expresses its partition between the air and water phases. It helps to predict the behavior of an organic compound in the environment and in remediation procedures such as air stripping processes. These values also describe the movement of a chemical from water to air and vice versa. High values mean that the chemical will move more toward the gas phase whereas low values indicate stronger partitioning into the aqueous phase (atm m^3/mole).

Conversion factor from dimensionless to other types of Henry's law constants:

= 4.034E-04	mol/(m^3Pa)
= 4.088E-02	M/atm
= 1.000E+00	(dimensionless aq/g)
= 4.046E-07	mol/(kg Pa)
= 4.100E-02	mol/(kg atm)
= 7.386E-04	1/atm
= 1.354E+03	atm
= 2.479E+03	m^3Pa/mol
= 1.000E+00	(dimensionless g/aq)
Source: http://www.mpch-mainz.mpg.de/~sander/cgi-bin/henry-conv/henry-conv.cgi?value=1&kHtype=kHccinv	

Henry's law constant temperature: The Henry's law constant temperature is the temperature corresponding to the Henry's law constant value (degree C).

Octanol-water partitioning coefficient (K_{ow}): This is a ratio of the equilibrium concentration of a dissolved substance in a system of two immiscible liquids–water and octanol. After a chemical has been mixed in an octanol and water solution, the system is allowed to reach equilibrium. The two phases will partition and a ratio of the concentration of the chemicals in the octanol and

water phases is taken. This ratio provides an indication of chemical accumulation in water. More polar compounds will tend to partition into the aqueous phase, thus have a low K_{ow}. This is also a measurement of the hydrophobicity of an organic. The more hydrophobic, the more the contaminant will adsorb to soil or organics or biomass and have a low solubility (mL/mL).

Organic carbon partition coefficient (K_{oc}): The carbon matter partition coefficient describes the partitioning of a chemical between the aqueous phase and organic material, such as that present in soil. The K_{oc} is used as a measure of the tendency for organics to be adsorbed by soil. It is largely independent of soil properties (mL/g).

Exposure Parameters

The following properties are used to estimate exposure and intake from contact with contaminants.

GI absorption fraction, insoluble: The GI absorption fraction is the fraction of a substance absorbed during passage through the gastrointestinal tract following ingestion. The value for insoluble material is used primarily for chemicals present in less soluble forms.

Aqueous skin permeability: The skin permeability constant (cm/hr) gives the rate of absorption of a chemical through the skin to the blood. It is used to evaluate the transfer of a chemical into the blood for situations involving contact with aqueous solutions of a chemical. Values range from 0 to 1.

Decay Rates

This group includes parameters that describe environmental decay rate processes, including loss rates from media, biodegradation, oxidation, hydrolysis, photolysis, and reaction rates.

Half-life in air: This is a general loss parameter used to describe the net loss rate of a chemical during air transport (days).

Half-life in soil: This is a general loss parameter used to describe the net loss rate of a chemical during transport in subsurface soil (days).

Half-life in groundwater: This is a general loss parameter used to describe the net loss rate of a chemical during groundwater transport (days).

Half-life in surface water: This is a general loss parameter used to describe the net loss rate of a chemical during surface water transport (days).

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)*	**2. REPORT TYPE**	**3. DATES COVERED** *(From - To)*
September 2002	Final report	

4. TITLE AND SUBTITLE

Compilation of Physical and Chemical Properties and Toxicity Benchmarks for Military Range Compounds

5a. CONTRACT NUMBER

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)

Mansour Zakikhani, Mark S. Dortch, Jeffrey A. Gerald

5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

U.S. Army Engineer Research and Development Center
Environmental Laboratory
3909 Halls Ferry Road
Vicksburg, MS 39180-6199

8. PERFORMING ORGANIZATION REPORT NUMBER

ERDC/EL TR-02-27

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)

U.S. Army Environmental Center
5179 Hoadley Road
Aberdeen Proving Ground, MD 21010-5401

10. SPONSOR/MONITOR'S ACRONYM(S)

11. SPONSOR/MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION / AVAILABILITY STATEMENT

Approved for public release; distribution is unlimited.

13. SUPPLEMENTARY NOTES

A CD-ROM containing the physicochemical properties for military range compounds accompanies this report.

14. ABSTRACT

The U.S. Army Environmental Center (USAEC) has developed a test program to identify and quantify the emissions that result from weapons firing and from the use of pyrotechnic devices. The test program is divided into three distinct areas: characterization of smoke and pyrotechnic emissions, a firing point emission study, and an exploding ordnance emission study. One of the tasks associated with this program was to develop a database of physicochemical properties for the chemicals of greatest concern to USAEC. The objective of this project was to identify available data on physical/chemical properties required for fate and transport modeling of chemicals typically associated with munitions and their respective emissions and to compile these data as well as associated toxicity benchmarks. The physicochemical properties were obtained from a variety of sources. For many of the chemicals on the USAEC list, sufficient data on some of the physicochemical properties could not be obtained. For these chemicals, the physicochemical properties may be estimated from other sources such as the U.S. Environmental Protection Agency's ASTER program or other estimation softwares such as EPI. The data sources from FRAMES, CHPPM, RAIS, PhysProp, and *Physical-Chemical Properties and Environmental Fate and Degradation Handbook* as well as toxicity benchmarks were integrated into a single Microsoft Access 2000 database. A database-user interface was developed to allow for easy comparison of physicochemical properties among the individual data sources and display the toxicological data for these chemicals. The database is very flexible, can be updated easily, and has several useful options including printing each page of data or each cited reference. The resulting database has applications for exposure and effects assessment for risk characterization of chemicals associated with munitions and their associated emissions.

15. SUBJECT TERMS

Database
Military range compound
Physicochemical data
Toxicological benchmark data

16. SECURITY CLASSIFICATION OF:			**17. LIMITATION OF ABSTRACT**	**18. NUMBER OF PAGES**	**19a. NAME OF RESPONSIBLE PERSON**
a. REPORT	**b. ABSTRACT**	**c. THIS PAGE**			**19b. TELEPHONE NUMBER** *(include area code)*
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED		79	