ERDC/EL TR-05-16

US Army Corps of Engineers ®
Engineer Research and Development Center

Data Gap Analysis and Database Expansion of Parameters for Munitions Constituents

Mark Dortch, Mansour Zakikhani, John Furey,
Richard Meyer, Scott Fant, Jeffrey Gerald,
Mohammad Qasim, Herb Fredrickson, Patricia Honea,
Howard Bausum, Karen Walker, and Mark Johnson

December 2005

Environmental Laboratory

ERDC/EL TR-05-16
December 2005

Data Gap Analysis and Database Expansion of Parameters for Munitions Constituents

Mark Dortch, Mansour Zakikhani, John Furey, Richard Meyer, Scott Fant, Jeffrey Gerald, Mohammad Qasim, Herb Fredrickson, and Patricia Honea

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

Howard Bausum, Karen Walker, and Mark Johnson

U.S. Army Center for Health Promotion and Preventive Medicine
5158 Blackhawk Road
Aberdeen Proving Ground, MD 21010-5403

Final report

Prepared for U.S. Army Corps of Engineers
Washington, DC 20314-1000

ABSTRACT: Training and munitions firing activities at military ranges are operations vital to the readiness of the U.S. Army. These activities involve the use of pyrotechnic, explosive, and incendiary compounds. During an initial effort, the U.S. Army Engineer Research and Development Center (ERDC) and the U.S. Army Center for Health Promotion and Preventive Medicine (CHPPM) developed a Range Database for 188 chemicals of range interest specified by the U.S. Army Environmental Center. Significant gaps existed in the initial database, which included 11 priority physicochemical properties and human toxicological benchmarks. In recognition of the substantial remaining data gaps in the Range Database, this study was conducted by ERDC and CHPPM to expand the database for additional properties and human exposure parameters and to fill data gaps to the extent possible, even to include computational or estimation methods, if appropriate. The study effort was divided into five property/parameter categories: physicochemical properties for fate and transport, human exposure parameters, food transfer factors, environmental degradation rates and half-lives, and human toxicological benchmarks. The accuracy of estimation methods was evaluated. Recommendations are made for estimation methods and future research to address any remaining data gaps or to improve estimates. The data are being added to a relational database.

.

Contents

List of Figures

List of Tables

Preface

This report describes the investigation of methods to estimate parameters used in human exposure and effects assessment associated with chemicals that may be released on Army training and firing ranges. These parameters include physicochemical properties, human exposure factors, human food transfer factors, environmental degradation rates, and human toxicological benchmarks. A range constituent database was expanded to include additional parameters and parameter estimates as discussed in this report.

This study was conducted by the U.S. Army Engineer Research and Development Center (ERDC) and the U.S. Army Center for Health Promotion and Preventive Medicine (CHPPM) through funding from the U.S. Army Environmental Center (AEC). Dr. Ira May of AEC was the Project Monitor, and Ms. Tamara L. Rush with Booz Allen Hamilton, a contractor for AEC, was the project coordinator.

This study was conducted by the following personnel: Drs. Mark Dortch, Research Civil Engineer, Mansour Zakikhani, Research Civil Engineer, Richard Meyer, Chemist, John Furey, Research Physical Scientist, Herb Fredrickson, Microbiologist, and Mohammad Qasim, Research Chemist, and Mr. Jeffrey Gerald, Research Physical Scientist, of the ERDC Environmental Laboratory (EL); Drs. Howard Bausum, Toxicologist, Karen Walker, Toxicologist, and Mark S. Johnson, Toxicologist, of CHPPM; and Ms. Patricia Honea, Contract Student, and Mr. Scott Fant, Research Scientist, of Analytical Services, Inc. (ASI), an onsite contractor for EL. Dr. Dortch was the project leader for the ERDC portion of the study, and Dr. Johnson was project leader for the CHPPM portion, which dealt with the human toxicological benchmarks. Dr. Dortch wrote Chapters 1 and parts of Chapters 2 and 9. Dr. Zakikhani contributed to Chapter 2 and wrote Chapters 4 and 5. Dr. Meyer wrote the sections of Chapter 3 dealing with the five physicochemical properties. Mr. Fant wrote the sections of Chapter 3 on diffusivity in air and water. Drs. Furey, Qasim, and Fredrickson wrote Chapter 6. Drs. Bausum, Walker, and Johnson wrote Chapter 7. Messrs. Gerald and Fant wrote Chapter 8. Drs. Dortch and Zakikhani conducted the technical editing.

COL James Rowan, EN, was Commander and Executive Director of ERDC. Dr. James R. Houston was Director.

1 Introduction

Background

Training and testing activities at military ranges are operations vital to the readiness of the U.S. Army. These activities involve the use of pyrotechnic, explosive, and incendiary compounds. Residues of these substances have been found in soil, air, surface water, and groundwater samples. Safeguarding the health of soldiers, civilians, and the environment requires an evaluation of the impact of these substances. These evaluations require knowledge of fate and transport of these substances in the environment as well as sound toxicological information to determine if exposures are safe.

The U.S. Army Environmental Center (AEC) has 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 task associated with this program is to develop a database with physicochemical properties, parameters for exposure assessment, and human toxicological benchmarks for chemicals found on ranges as listed by AEC.

During an initial effort (Zakikhani et al. 2002), the U.S. Army Engineer Research and Development Center (ERDC) and the U.S. Army Center for Health Promotion and Preventive Medicine (CHPPM) developed a database for 188 chemicals specified by AEC. That database was limited to 11 primary physicochemical properties/exposure parameters and 12 human toxicological benchmarks since measured and reliable values for other properties were not readily available. Techniques are available to estimate some properties and parameters, but such estimations border on a research effort that exceeded the scope of the initial effort. An analysis of the availability of physicochemical properties/parameters in the initial database indicated that only 13 percent of chemicals in the list have data for all 11 properties/parameters; 30 percent of chemicals have data only for 10 properties/parameters; and 3 percent of chemicals in the list do not have any property/parameter values in the database. In general, significant gaps existed in the initial database for the first 11 properties/parameters and toxicological benchmarks, as well as major gaps in data for other parameters needed for fate/transport and exposure assessment.

The Range Database is one of several constituent databases used by the Adaptive Risk Assessment Modeling System (ARAMS). ARAMS (http://el.erdc.usace.army.mil/arams/) was developed by ERDC and CHPPM under the Army's Environmental Quality Technology Program. In addition to the Range Database, ARAMS has the FRAMES (http://mepas.pnl.gov/FRAMESV1/paramete.html) constituent database, and a link is being developed to the Risk Assessment Information System (RAIS) constituent database (http://risk.lsd.ornl.gov/index.shtml). The Range Database focuses on constituents expected on firing and training ranges, whereas the ARAMS/FRAMES and RAIS databases include a diverse list of chemicals and radionuclides.

In recognition of the substantial remaining data gaps for the Range Database, AEC requested CHPPM and ERDC to conduct this study in an attempt to expand the database for additional properties and parameters and to fill gaps to the extent possible, and to include computational or estimation methods if appropriate. This report presents the results of this follow-up study and identifies remaining gaps with recommendations for addressing those gaps.

The terms "property" and "parameter" may appear to be used interchangeable in this report. For clarification, a property is considered a physicochemical characteristic, such as molecular weight or octanol to water partition coefficient. A parameter is an environmental coefficient used to describe some process, such as environmental degradation rates, food transfer factors, and gastrointestinal absorption fraction. However, in this report, the term "parameter" may be used more often in a general sense to denote all of the variables of interest, including physicochemical properties, exposure parameters, and toxicological benchmarks.

Objectives

The overall objective of this study was to expand the database to fill data gaps for the parameters already in the database and to add additional priority parameters and associated data to the database. The challenge was to fill as many data gaps as feasible within the budgetary and technological constraints for the full list of range chemicals. It was recognized from the beginning that in order to make significant progress on filling these gaps, it would be necessary to resort to computational methods, extrapolation, and other means for estimating parameter values. Therefore, a major part of this study was devoted to evaluating and recommending various methods for predicting parameter values, then using such methods to generate parameter estimates for the database. Objectives included documenting the accuracy of recommended estimation techniques, expanding the database to include new values, and documenting remaining data gaps.

Scope of Work

The study consisted of basically four steps: evaluation of estimation methods; generation of parameter values; database expansion; documentation of results; and identifying data gaps as presented in this report. This study did not preclude additional searches for parameter values in the literature as done in the first study, but with the number of chemicals and parameters, it was not possible to focus exhaustive attention to such searches. Thus, most of the emphasis of this study was placed on the use of parameter estimation methods. Additionally, this study was limited in scope to only those parameters needed for human exposure and effects assessment, but included parameters for fate and transport that may be part of exposure assessment. However, there was no effort devoted to ecological exposure parameters beyond fate and transport.

The study effort was distributed among the investigators according to the following parameter categories:

- Physicochemical properties for fate and transport.
- Human exposure parameters.
- Food transfer factors.
- Environmental degradation rates.
- Human toxicological benchmarks.

The ERDC focused on the first four parameter categories, and CHPPM focused on the fifth--human toxicological benchmarks. ERDC was responsible for revising the Range Database.

For each of the above parameter categories, the investigator surveyed available methods for estimating the parameters within the category, analyzed the accuracy of the recommended methods, generated estimates for parameter values, assessed remaining data gaps, and provided recommendations. The remainder of this report follows this general outline, and there is a chapter for each of the five parameter categories. Chapter 2 presents the chemicals and parameters under study. Chapters 3-7 cover each of the five parameter categories listed above in that order. Chapter 8 describes the format or schema for the revised Range Database. Chapter 9 provides a summary of conclusions and recommendations.

2 Chemicals, Parameters, and Statistical Methods

Chemicals of Concern

The chemicals of interest for Army training and firing ranges were provided by AEC and are listed in Table 1. The Chemical Abstract Service (CAS) registry number is also listed for each chemical in Table 1 along with the chemical class (termed group, as discussed below). The assignment of the compounds of interest to various classes was completed on the basis of a review of each compound's structure and subsequent identification of its most important functional group or moiety. Because compounds containing the same functional group normally exhibit similar physical and chemical properties, this type of classification results in the grouping of compounds that would be expected to have similar environmental impacts into a single class set. In those cases where no single dominant functional group is present, the compound was identified by its most common use (e.g. a dye). In those few instances where compounds were the only member of an uncommon functional group class, they were either placed into a closely related group or else into the group "other."

Table 1
List of Chemicals of Interest

ID	Chemicals	CAS Number	Group or Class
1	1,2-dichloroethene (cis)	156-59-2	halogenated
2	1,2-dichloroethene (trans)	156-60-5	halogenated
3	(1,2-dichloroethyl) benzene	1074-11-9	halogenated
4	1,2,4-trimethylbenzene	95-63-6	hydrocarbons
5	1,2-dichlorethane	107-06-2	halogenated
6	1,2-dichloro-3-methylbenzene	32768-54-0	halogenated
7	1,2-dichloroethene (cis/trans mixture)	540-59-0	halogenated
8	1,3,5-trimethylbenzene (mesitylene)	108-67-8	hydrocarbons
9	1,3,5-trinitrobenzene	99-35-4	explosives
10	1,3-butadiene	106-99-0	hydrocarbons
11	1,3-dinitrobenzene	99-65-0	explosives
12	1,4-diamino-2,3-dihydroanthraquinone (DDA) violet-dye mix	81-63-0	biocides/dyes
13	1,4-di-p-toluidinoanthraquinone (PTA) solvent green 3	128-80-3	biocides/dyes
14	1-butanol	71-36-3	alchohols/ketones
15	1-butene	106-98-9	hydrocarbons
16	1-chloro-2-methylbenzene	95-49-8	halogenated
17	1-chloro-3-methylbenzene	108-41-8	halogenated

(Sheet 1 of 4)

Table 1 (Continued)

ID	Chemicals	CAS #Number	Group or Class
18	1-hexene	592-41-6	hydrocarbons
19	1-pentene	109-67-1	hydrocarbons
20	1-(methylamino)anthraquinone (disperse red 9)	82-38-2	biocides/dyes
21	2-(2-quinolyl)-1,3-indandione (D & C yellow no. 11) or (solvent yellow 33)	8003-22-3	biocides/dyes
22	2,3-butanedione	431-03-8	alcohols/ketones
23	2,3,7,8-tetrachlorodibenzo-p-dioxin	1746-01-6	furans+dioxins
24	2,4,6-trinitrotoluene (TNT)	118-96-7	exploosives
25	2,4-dinitrotoluene (DNT; 2,4-DNT)	121-14-2	exploosives
26	2,6-dinitrotoluene (2,6-DNT)	606-20-2	exploosives
27	2,5-dimethylfuran	625-86-5	furans+dioxins
28	2-amino-4,6-dinitrotoluene	35572-78-2	exploosives
29	2-amino-9,10-anthracenedione (a) (AAQ)	117-79-3	biocides/dyes
30	2-butanone	78-93-3	alcohols/ketones
31	2-furaldehyde	98-01-1	alcohols/ketones
32	2-heptanone	110-43-0	alcohols/ketones
33	2-methyl-1-butene	563-46-2	hydrocarbons
34	2-methylfuran	534-22-5	furans+dioxins
35	2-methylthiophene	554-14-3	hydrocarbons
36	2-nitrotoluene (ONT)	88-72-2	exploosives
37	2-pentanone	107-87-9	alcohols/ketones
38	2-propanol	67-63-0	alcohols/ketones
39	2-thiophenecarboxaldehyde	98-03-3	alcohols/ketones
40	3-(phenylhydrazone)-1H-indole-2,3-dione	17310-26-8	other
41	3-furaldehyde	498-60-2	alcohols/ketones
42	3-methyl-1-butene	563-45-1	hydrocarbons
43	3-methylfuran	930-27-8	furans+dioxons
44	3-methylthiophene	616-44-4	hydrocarbons
45	3-nitrotoluene	99-08-1	explosives
46	4-1,2,4-oxadizaolin-3-one-2,5-diphenyl-delta	unknown	unknown
47	4-amino-2,6-dinitrotoluene (4ADNT)	19406-51-0	explosives
48	4-ethyltoluene	622-96-8	hydrocarbons
49	4-methyl-2-pentanone	108-10-1	alcohols/ketones
50	4-nitrotoluene	99-99-0	explosives
51	4-phenoxy-2(1H)-quinolinone	66662-28-0	biocides/dyes
52	acenaphthene	83-32-9	PAHs+PCBs
53	acenaphthylene	208-96-8	PAHs+PCBs
54	acetaldehyde	75-07-0	alcohols/ketones
55	acetic acid	64-19-7	alcohols/ketones
56	acetone	67-64-1	alcohols/ketones
57	acetonitrile	75-05-8	hydrocarbons
58	acetophenone	98-86-2	alcohols/ketones
59	acetylene	74-86-2	hydrocarbons
60	acrolein	107-02-8	hydrocarbons
61	acrylonitrile	107-13-1	hydrocarbons
62	aluminum	7429-90-5	metals/inorganics
63	anthracene	120-12-7	PAHs+PCBs
64	antimony	7440-36-0	metals/inorganics
65	arsenic	7440-38-2	metals/inorganics
66	barium	7440-39-3	metals/inorganics
67	benzaldehyde	100-52-7	alcohols/ketones
68	benzanthrone (b)	82-05-3	biocides/dyes
69	benzene	71-43-2	hydrocarbons
70	benzo(a)anthracene	56-55-3	PAHs+PCBs
71	benzo(a)pyrene	50-32-8	PAHs+PCBs
72	benzo(b)fluoranthene	205-99-2	PAHs+PCBs
73	benzo(e)pyrene	192-97-2	PAHs+PCBs
74	benzo(g,h,i)perylene	191-24-2	PAHs+PCBs
75	benzo(k)fluoranthene	207-08-9	PAHs+PCBs

(Sheet 2 of 4)

Table 1 (Continued)

ID	Chemicals	CAS Number	Group or Class
76	benzofuran	271-89-6	furans+dioxins
77	benzonitrile	100-47-0	biocides/dyes
78	beryllium	7440-41-7	metals/inorganics
79	bis(2-ethylhexyl)phthalate	117-81-7	hydrocarbons
80	butanal	123-72-8	alcohols/ketones
81	cadmium	7440-43-9	metals/inorganics
82	calcium	7440-70-2	metals/inorganics
83	carbon dioxide (CO2)	124-38-9	gases
84	carbon disulfide	75-15-0	gases
85	carbon monoxide (CO)	630-08-0	gases
86	carbon tetrachloride	56-23-5	halogenated
87	carbonyl sulfide	463-58-1	gases
88	chlorobenzene	108-90-7	halogenated
89	chloroethene (vinyl chloride)	75-01-4	halogenated
90	chloroform	67-66-3	halogenated
91	chloromethane	74-87-3	halogenated
92	chromium	7440-47-3	metals/inorganics
93	chrysene	218-01-9	pahs+pcbs
94	cis-2-butene	590-18-1	hydrocarbons
95	Cl2 (a)	7782-50-5	gases
96	cobalt	7440-48-4	metals/inorganics
97	copper	7440-50-8	metals/inorganics
98	dibenz(a,h)anthracene	53-70-3	pahs+pcbs
99	dibenzo(b,def)chrysene-7,14 dione (c.i. vat yellow 4)	128-66-5	biocides/dyes
100	dibutyl phthalate	84-74-2	hydrocarbons
101	dichloroacetonitrile	3018-12-0	halogenated
102	dichlorodiflouromethane	75-71-8	halogenated
103	dimethyltrisulfide	3658-80-8	gases
104	diphenylamine	122-39-4	biocides/dyes
105	ethane	74-84-0	hydrocarbons
106	ethanol	64-17-5	alcohols/ketones
107	ethyl benzene	100-41-4	hydrocarbons
108	ethyl chloride	75-00-3	halogenated
109	ethylene	74-85-1	hydrocarbons
110	fluoranthene	206-44-0	pahs+pcbs
111	fluorene	86-73-7	pahs+pcbs
112	formaldehyde	50-00-0	alcohols/ketones
113	furan	110-00-9	furans+dioxins
114	HCl	7647-01-0	other
115	heptanal	111-71-7	alcohols/ketones
116	hexachlorobenzene	118-74-1	halogenated
117	hexachlorobutadiene	87-68-3	halogenated
118	hexachlorocyclopentadiene	77-47-4	halogenated
119	hexachloroethane	67-72-1	halogenated
120	hexanal	66-25-1	alcohols/ketones
121	hexane	110-54-3	hydrocarbons
122	HMX	2691-41-0	explosives
123	hydrogen cyanide	74-90-8	biocides/dyes
124	i-butane (isobutane)	75-28-5	hydrocarbons
125	i-butene (isobutene/e-butylene)	115-11-7	hydrocarbons
126	indeno(1,2,3-cd)pyrene	193-39-5	pahs+pcbs
127	isothiocyanatomethane	556-61-6	biocides/dyes
128	lead	7439-92-1	metals/inorganics
129	xylene (mixed isomers)	1330-20-7	hydrocarbons
130	m-xylene (meta-xylene)	108-38-3	hydrocarbons
131	p-xylene (para-xylene)	106-42-3	hydrocarbons

(Sheet 3 of 4)

Table 1 (Concluded)

ID	Chemicals	CAS Number	Group or Class
132	magnesium	7439-95-4	metals/inorganics
133	manganese	7439-96-5	metals/inorganics
134	m-dichlorobenzene	541-73-1	hydrocarbons
135	mercury	7439-97-6	metals/inorganics
136	methacrolein	78-85-3	PAHs+PCBs
137	methane	74-82-8	hydrocarbons
138	methylene chloride	75-09-2	halogenated
139	methylnitrite	624-91-9	explosives
140	methyl-t-butylether (MTBE)	1634-04-4	alcohols/ketones
141	methyl-vinyl ketone	78-94-4	alcohols/ketones
142	naphthalene	91-20-3	PAHs+PCBs
143	n-butane	106-97-8	hydrocarbons
144	n-decane	124-18-5	hydrocarbons
145	NH3 (ammonia)	7664-41-7	gases
146	nickel	7440-02-0	metals/inorganics
147	nitric acid	7697-37-2	other
148	nitrobenzene	98-95-3	explosives
149	nitrogen oxide (NOx)	10102-44-0	gases
150	nitroglycerine	55-63-0	explosives
151	nitromethane	75-52-5	explosives
152	nonanal	124-19-6	alcohols/ketones
153	OCDD (1,2,3,4,6,7,8,9-OCDD)	3268-87-9	furans+dioxins
154	octanal	124-13-0	alcohols/ketones
155	o-dichlorobenzene	95-50-1	halogenated
156	o-methoxy-phenyl-azo-b-naphthol (oil red g)	1229-55-6	biocides/dyes
157	o-xylene (ortho-xylene)	95-47-6	hydrocarbons
158	particulate cyanide	57-12-5	biocides/dyes
159	p-dichlorobenzene (para-dichlorobenzene)	106-46-7	halogenated
160	pentaerythritoltetranitrate (PETN)	78-11-5	explosives
161	perchloroethylene	127-18-4	halogenated
162	phenanthrene	85-01-8	PAHs+PCBs
163	phenol	108-95-2	alcohols/ketones
164	phenylacetylene (ethynyl benzene)	536-74-3	hydrocarbons
165	phosphorus	7723-14-0	metals/inorganics
166	propanal	123-38-6	alcohols/ketones
167	propane	74-98-6	hydrocarbons
168	propylene	115-07-1	hydrocarbons
169	propyne	74-99-7	hydrocarbons
170	pyrene	129-00-0	PAHs+PCBs
171	RDX	121-82-4	explosives
172	selenium	7782-49-2	metals/inorganics
173	silver	7440-22-4	metals/inorganics
174	styrene (vinyl benzene)	100-42-5	hydrocarbons
175	sulfur dioxide (SO2)	7446-09-5	gases
176	sulfuric acid	7664-93-9	other
177	tetryl (2,4,6-trinitrophenylmethylnitramine)	479-45-8	explosives
178	thallium	7440-28-0	metals/inorganics
179	thiophene	110-02-1	hydrocarbons
180	toluene	108-88-3	hydrocarbons
181	trans-2-butenal	123-73-9	alcohols/ketones
182	trans-2-butene	624-64-6	hydrocarbons
183	trans-2-pentene	646-04-8	hydrocarbons
184	trans-3-penten-2-one	625-33-2	alcohols/ketones
185	trichloroethylene (TCE)	79-01-6	halogenated
186	trichlorofloUromethane	75-69-4	halogenated
187	vinylidenechloride	75-35-4	halogenated
188	zinc	7440-66-6	metals/inorganics

(Sheet 4 of 4)

The original list from AEC included 195 chemicals, but the chemical list used in this study has 188 chemicals because repeated chemicals were removed from the list (Table 1). For 187 chemicals listed in Table 1, CAS numbers were identified, but for one chemical, 4-1,2,4-oxadizaolin-3-one-2,5-diphenyl-delta, the CAS number could not be determined; thus, no information was sought for this compound (and it is classified as "unknown").

Parameters

The parameters of interest for exposure assessment generally include those for fate/transport, human exposure pathways, food transfer factors for humans, and environmental degradation rates. The primary parameters of interest for these four categories are listed in Table 2 where the list in Table 2 was taken from the FRAMES constituent data base (http://mepas.pnl.gov/FRAMESV1/paramete.html). The human toxicological benchmarks in Table 2 that are used for effects assessment were also considered in this study. Table 2 does not include process rates such as dissolution rate. Process rates generally depend on parameters or properties such as those in Table 2. Several parameters/properties in Table 2 were not addressed in this study as indicated.

Table 2
Chemical Parameters and Properties

Physical properties and partitioning used for fate/transport	Not Addressed in the Study
Molecular weight, g/mole	
Octonol-water partition coefficient (K_{ow}), L/kg	
Water solubility, mg/L	
Water solubility reference temperature, °C	
Vapor pressure, mm Hg	
Vapor pressure reference temperature, °C	
Henry's law constant, atm m^3/mole	
Henry's law constant reference temperature, °C	
Organic carbon partition coefficient (K_{oc}), L/kg	x
Soil-water distribution coefficient for inorganics (K_d), L/kg	x
Molecular diffusivity in air and water, cm^2/sec	
Human exposure factors	
Aqueous skin permeability, cm/hr	
GI absorption fraction (GI ABS)	
Dermal absorption fraction from soil	
Human food transfer factors (aquatic, animal, and plant)	
Bioaccumulation in freshwater fish, L/kg	
Bioaccumulation in freshwater mollusk, L/kg	x
Bioaccumulation in freshwater crustacea, L/kg	x
Bioaccumulation in freshwater plants, L/kg	x
Bioaccumulation in saltwater fish, L/kg	x
Bioaccumulation in saltwater mollusk, L/kg	x
Bioaccumulation in saltwater crustacea, L/kg	x
Bioaccumulation in saltwater plants, L/kg	x
Feed to animal meat transfer factor, day/kg	

(Continued)

Table 2 (Concluded)

Human food transfer factors (aquatic, animal, and plant) (Continued)	Not Addressed in the Study
Feed to animal milk transfer factor, day/L	
Feed to poultry transfer factor, day/kg	
Feed to pork transfer factor, day/kg	
Feed to egg transfer factor, day/kg	
Soil to plant concentration ratio for leafy vegetables, kg soil/kg (dry)	
Soil to plant concentration ratio for root vegetables, kg soil/kg (dry)	
Soil to plant concentration ratio for fruit, kg soil/kg (dry)	
Soil to plant concentration ratio for cereal, kg soil/kg (dry)	
Soil to plant concentration ratio for animal forage, kg soil/kg (dry)	
Soil to plant concentration ratio for hay, kg soil/kg (dry)	
Soil to plant concentration ratio for grain, kg soil/kg (dry)	
Soil to plant concentration ratio, other vegetables, kg soil/kg (dry)	
Root concentration factor, mg/kg per mg/kg	
Air to plant transfer factor for leafy vegetables, mg/kg per mg/kg	
Air to plant transfer factor for forage, mg/kg per mg/kg	x
Environmental degradation rates or half-lives	
Half time in air (process not specified)	
Half time in groundwater (process not specified)	x
Half time in surface water (process not specified)	
Half time in soil or sediment (process not specified)	
Oxidation half-lives in air	
Hydrolysis half-lives in water	x
Photodegradation half-lives in air	x
Photodegradation half-lives in water	x
Biodegradation half-lives in air	x
Biodegradation hal-lives in water	
Biodegradation half-lives in soil	
Human toxicological benchmarks	
Inhalation cancer potency factor, $(mg/kg/day)^{-1}$	
Oral cancer potency factor, $(mg/kg/day)^{-1}$	
Inhalation reference dose, mg/kg/day	
Oral reference dose, mg/kg/day	
Inhalation unit risk, $(mg/m^3)^{-1}$	x
Inhalation reference concentration, mg/m^3	x
Oral unit risk, $(mg/L)^{-1}$	x

Statistical Methods

Statistical techniques may be used to evaluate the quality of estimates for chemical properties. Various statistics that have been used to evaluate model accuracy or error relative to observed data are described below. Subsets of some of the data presented in this report were analyzed with the various statistics to determine which statistics would be best to use for evaluating the accuracy of various property estimation methods.

1. Root mean square error (rmse) is an estimate of the pooled variability of the model predictions and the observed data. The lowest rmse is an indication of the "best" model. However, rmse will not be a good indicator unless the model variance and the observed data variance are

similar in magnitude. In the half-life data, the observed data variance (10^{15}) dwarfs the model variance (10^4 to 10^6), so rmse should not be used unless the data cleanup and subsetting bring the variances closer to each other. The rmse has a lower bound of zero and no specific upper bound.

$$\text{rmse} = \sqrt{\frac{\sum (s_i^2 (n_i - 1))}{\sum (n_i - 1)}} \quad (1)$$

where s_i^2 and n_i are the variance and number of observations, respectively, of data set *i*.

2. The regression coefficient of determination, R^2, is a measure of the variability explained by the regression model of predicted data vs. observed data. The model with the highest R^2 indicates the best fit of predicted to observed values. Low R^2 values indicate poor linear fit and poor predictive ability. Note that for ordinary regression, R^2 is a measure of *linear* association only. Data cleanup and sub-setting may help to improve linearity. In some cases, data transformation (e.g. logarithms) of one or both variables may help to establish linearity. Alternatively, a nonlinear regression model may be used. R^2 is bounded between 0 and 1.

3. Average prediction relative error is a metric that standardizes the residuals to the observed data. Lower positive average predicted relative error indicates less discrepancy between predicted and observed data.

$$\text{avg pred rel err} = \frac{\sum [(\text{pred} - \text{obs})/\text{obs}]}{n} \quad (2)$$

The relative error is bounded by a lower limit of -1 and an upper limit approaching the predicted value. When the observed value is zero, the relative error is undefined. The average predicted relative error could be very difficult to interpret in a situation where it was negative for one model (constrained between –1 and 0) and positive for another model (where predicted is the only upper constraint).

4. Average absolute residuals is an unstandardized measure of the non-directional magnitude of discrepancy between predicted and observed data, where

$$\text{avg abs resid} = \frac{\sum |(\text{pred} - \text{obs})|}{n} \quad (3)$$

The "best" model will have the lowest average absolute residual. The residuals have no specific bounds other than the data themselves. This metric will be profoundly influenced by any outliers that cause huge discrepancies.

5. Average bias is a directional measure of the average magnitude of discrepancy between predicted and observed data:

$$\text{avg bias} = \frac{\sum(\text{pred} - \text{obs})}{n} \quad (4)$$

Its usefulness lies in quantifying the tendency of the model predictions to either overestimate or underestimate the observed data. The "best" model will have bias closest to zero. Along with bias, it would be useful to report the proportion of compounds for which the model prediction overestimates or underestimates the observed value.

6. Average model error (AME), also absolute mean error, is a standardized measure of model uncertainty expressed as a percent of the observed value. AME cannot be calculated when the observed value = 0. AME is calculated as

$$\text{AME} = \frac{100 \sum \left| \frac{\text{obs} - \text{pred}}{\text{obs}} \right|}{n} \quad (5)$$

Unlike average predicted relative error, the AME has a lower bound of zero, and as a percent is intuitively easy to compare among models.

The AME and average bias seemed to best accommodate the needs of this study. Thus, these two statistical formulations were used to evaluate the accuracy of various estimation methods.

3 Physicochemical Properties for Fate and Transport

Introduction

The term "fate and transport" is, in general, referred to as the outcome of a contaminant in the environment as a result of its potential to be transported, transformed (physically, chemically, or biologically), or accumulated in one or more media. The environmental fate and transport of a contaminant is controlled by the compound's physical and chemical properties and the nature of the media through which the compound is migrating. Specific physicochemical parameters of interest are listed in Table 2 (Chapter 2). The parameters addressed in this chapter are: 1) molecular weight, 2) octanol-water partition coefficient (K_{ow}), 3) water solubility, 4) vapor pressure, 5) Henry's law constant, and 6) molecular diffusivity in air and water. This chapter describes the data analysis of the five physicochemical properties first and then the analysis of diffusion coefficients.

The organic carbon partition coefficient and the soil-water distribution coefficient for inorganic constituents were not addressed in this study. The organic carbon partition coefficient is not usually necessary if K_{ow} is known because it is usually estimated from K_{ow}. Soil-water distribution coefficients (K_d) for inorganic chemicals are chemical- and media-specific. The development of generally applicable relationships for estimating inorganic K_d values has been an illusive, long-term endeavor and is beyond the scope of this study. However, compilation of observed values has resulted in some information on K_d for inorganic chemicals and radionuclides (Strenge et al. 1989). This compilation is in the form of a look-up table as related to soil pH and composition (percent total weight of clay, organic mater, and iron and aluminum oxyhydroxides). This look-up table functionality is built into ARAMS/FRAMES for the models that require K_d. Values of K_d for organic chemicals can be estimated from relationships involving K_{ow} and soil composition.

Five Physicochemical Properties

Methods

Most of the compounds in Table 1 do not have complete measured sets of property values, and, therefore, computationally based methods were used to estimate physical properties for those compounds. The primary technique employed in providing estimates of those properties not otherwise available was the quantitative structure activity relationship (QSAR) and the quantitative structure property relationship (QSPR). Because both QSAR and QSPR use compounds with known properties to establish relationships between structure and either activity or physical properties, it was necessary to have a linked set of compound structures and properties. A database of this information is referred to as a training set. Any training set that is to be utilized as a basis for property predictions in the QSAR/QSPR approach either must be from a previously trained data set or be constructed from a well-behaved training set.

The process of using QSAR/QSPR requires that all compounds have known structures and that these structures be provided in a format that can be used either in establishing a training set (for compounds with known properties) or to estimate a property (for compounds with unknown properties). The basic premise of QSAR/QSPR is that by considering a significant number of different compounds with known property values, molecular fragmentation techniques can be employed to identify property-structure relationships. With sufficient training, it is possible to extend the gross property-structure dependence that is observed to a quantitative and predictive relationship. The process works as follows: numerous compounds with known property values are analyzed, and it is determined when the particular structure "fragment A" is found in a compound with a definite correlation to the property of interest. Further, with an appropriate training set, it may be possible to link the presence of "fragment A" with a quantitative contribution to a physical property such as the octanol-water partition coefficient. In order to accurately estimate a physical property using QSAR/QSPR, it is necessary to have the ability to associate as many of the structures found in a compound as possible with the appropriate quantitative contributions for the physical property of interest. This process normally requires the use of computer programs to identify and evaluate the quantitative relationships contained in a training set. For the purposes of this study, the primary software tool used was the QSAR Builder (QB) software from Pharma Algorithms (Pharma Algorithms Inc., QSAR Builder v 1.6, www.ap-algorithms.com).

The chemicals of interest (Table 1) were evaluated for the presence of existing published data on the properties of interest. The results of the review of existing references (Chemical and Physical Properties Database, http://www.dep.state.pa.us/physicalproperties/; IUPAC-NIST Solubility Database, Version 1.0, http://srdata.nist.gov/solubility/; and Sander (1999), http://www.mpch-mainz.mpg.de/~sander/res/henry.html) yielded peer reviewed property values in approximately half of the compounds. Those property values that were found provided material for the training set data that was used in the

QSAR/QSPR modeling phase of the project. In the compilation of the existing property values, it was often necessary to determine which value of a historical data set to include in the training data. In those instances where multiple values were found, a preference was given to empirically derived and recently published values. The number of instances of multiple reported values with significant differences among the values was rare.

The minimized bonded structures for the chemicals of interest (Table 1) were prepared using the GaussView (GV) software from Gaussian, Inc. (Semichem, Inc., GaussView v 3.0.9, www.gausian.com). All structures were prepared manually within the GV software and were then adjusted to an approximately optimized structure using the built-in "Clean" function (default settings were used) within GV. Further, structural optimizations were not required for the QSAR/QSPR studies as the QSAR software uses relative (i.e. adjacent fragment, fragment one group removed, etc.), not absolute positions to build its interaction matrices. Whenever possible, the prepared chemical structures were compared to the structural information contained within the National Institute of Standards and Technology (NIST) spectral database (NIST Mass Spectral Standard Reference Database 1A) and verified for correctness of bond length and strengths. Once the structures were completed, they were converted from the native Gaussian input file format and saved in the MDL MOL-file (.mol) format for input into the QB software.

The structures generated were each individually imported into the QB program where they were automatically assigned a QB database identification number and used to form the basis of a project database. Each compound was then identified within the project database with its unique CAS number, a compound name, and its assigned compound type. The additional information initially loaded into the QB database (not including the actual structure) was for identification purposes. The compound type entry was used to group various chemical families for the QSAR/QSPR training.

The first property determined was the molecular mass of each compound; however, since most scientists still prefer to use the older term molecular weight (instead of the correct term mass), we will use that term here. The molecular weight (MW) was determined using the QB MW calculator which uses the straightforward procedure of identifying the number and type of each atom found in the molecular structures in the database, multiplying the determined number of atoms by the appropriate atomic mass (for the naturally occurring isotopic distribution of each element), and summing the products.

The octanol-water partition coefficient was calculated using a fragmental approach (Japertas et al. 2002, Mannhold and Dross 1996). This function is part of the QB and is based on a training set of greater than 9,800 compounds.

For approximately half of the compounds of interest, solubility constants were found to be published (Chemical and Physical Properties Database, http://www.dep.state.pa.us/physicalproperties/; and IUPAC-NIST Solubility Database, Version 1.0, http://srdata.nist.gov/solubility/). These known data for solubility were input into the QB database and modeled as one training set (due

to the limited numbers) to determine if a training set could be constructed from this available information. Based on the lack of correlation for the solubility constants when taken as a whole, which could not be improved by using smaller, more homologous groupings of data, it was concluded that, to predict solubility constants successfully, the training set needs to be increased significantly in the number of compounds that it contains. The remaining solubility constants were estimated using the ADME Boxes Solubility module software from Pharma Algorithms (Pharma Algorithms Inc., ADME Boxes v 2.2 (solubility), www.ap-algorithms.com). The Solubility module from Pharma Algorithms is based on a training set of more than 6,500 compounds.

For many (approximately two-thirds) of the compounds of interest, Henry's law constants (HLCs) were found to be published (IUPAC-NIST Solubility Database, Version 1.0, http://srdata.nist.gov/solubility/; Sander (1999), http://www.mpch-mainz.mpg.de/~sander/res/henry.html). These known HLC data were input into the QB database and initially modeled as one set to determine if a training set could be constructed from all the available information. Based on the lack of correlation for the HLCs when taken as a whole, it was determined that it would be necessary to group the existing data into a number of homologous groupings in an attempt to form predictive tools for specific compound types. The two largest subgroups available in the database for use as training sets, which also contained compounds without HLCs, were hydrocarbons (compounds with only carbon and hydrogen present) and oxygen containing hydrocarbons (compounds with only carbon, hydrogen, and oxygen present). These two subgroups were modeled to determine if a successful training set could be constructed from them individually. The results were such that although the training set gave a much improved correlation, it did not provide for accurate prediction of values. At the present time, no large training set exists for HLCs; therefore, in order to successfully predict HLCs, the training set needs to be increased significantly in the number of compounds that it contains. Such an expansion of the training set is beyond the scope of this project.

Estimates of the HLCs and the vapor pressures for each organic compound were completed using the U.S. Environmental Protection Agency's (USEPA's) and the University of Georgia's jointly developed SPARC software (SPARC Performs Automated Reasoning in Chemistry, http://www.epa.gov/athens/research/projects/sparc/ and http://ibmlc2.chem.uga.edu/sparc/). All SPARC estimates were completed for the conditions of 25 °C and 760 mm Hg pressure.

Analysis

All methods used for estimation/calculation of the properties of interest were evaluated using reference property values. In the case of the LogP (K_{ow}) and solubility properties, the SPARC program results were used as reference values; and for the vapor pressure and HLC, estimations from the SPARC program were compared to existing database values. Results of the statistical analysis providing both the average bias (Equation 4) and the AME (Equation 5) are listed in Table 3. Molecular weights (MW) were not included in Table 3 comparisons

as each MW was compared to the existing values in the ARAMS v1.5 database and were found to be identical within the level of precision expressed by the number of significant figures reported.

Table 3
Statistical Model Evaluation

Parameter	Units	Number of Comparisons	Average Bias	AME
LogP, (K_{ow})	Log(unitless)	137	0.237	67.1%
Log(*Sw*), Solubility	Log(mg/mL)	136	0.051	93.6%
Vapor pressure	Log(atm)	79	0.040	29.9%
Henry's law constant	Log(atm/(mol/m^3))	91	0.026	29.8%

Average bias gives a measure of the average difference between the values predicted (*pred)* by the method being used and the reference or observed (*obs*) value of the property. The evaluation of average bias also provides information on the tendency of the method being evaluated to under or over estimate relative to the reference set of values for the property of interest.

The AME provides a relative measure of the percent error in predicted/ calculated values relative to the reference values and gives a measure of the uncertainty in the model. AME has a lower limit of zero, and its result can be used to compare the uncertainty of different models.

Because the property values being calculated and/or estimated have such a large range of possible values (e.g. 20 orders of magnitude for vapor pressure), comparisons were computed using the typically logarithmically reported values.

Results

The statistical analysis of the various models utilized indicates a fairly good agreement in the values that are predicted. When the absolute range of values (12 orders of magnitude for the K_{ow} and up to 20 orders of magnitude for the vapor pressure values) is considered, the model errors appear relatively small: on the average, all predictions are within one order of magnitude of the reference values. Calculated or estimated values for the Range Database chemicals are summarized in Table 4. As shown in the table, for some chemicals values are not provided. For example, metals (in pure metallic form) are essentially insoluble in water, so they will not have either a K_{ow} or HLC. In addition, pure metals with the single exception of mercury do not have any appreciable vapor pressure. For a small number of the organic compounds (mixtures and/or functionally unique structures), it was not possible to estimate certain properties due to the limitations of the methods being used.

Table 4
Summary of Calculated or Estimated Values for Range Database Chemicals

Compound	CAS Number	MW g/mole	LogP (K_{ow}) Log()	Solubility Log(mg/mL)	Vapor Pressure Log(atm)	Henry's Law Log(atm/(mol/m^3))
1,2-dichloroethene (cis)	156-59-2	96.9426	2.25	-1.84	-0.26	-1.88
1,2-dichloroethene (trans)	156-60-5	96.9426	2.25	-1.84	-0.26	-1.88
(1,2-dichloroethyl) benzene	1074-11-9	175.0542	3.19	-3.82	--[1]	--[1]
1,2,4-trimethylbenzene	95-63-6	120.1911	3.44	-3.47	-2.53	-2.47
1,2-dichlorethane	107-06-2	98.9584	1.72	-1.65	-0.91	-2.81
1,2-dichloro-3-methylbenzene	32768-54-0	161.0277	3.72	-3.75	-3.23	-2.78
1,2-dichloroethene (cis/trans mixture)	540-59-0	96.9426	--[1]	--[1]	--[1]	--[1]
1,3,5-trimethylbenzene (mesitylene)	108-67-8	120.1911	3.44	-3.47	-2.41	-2.31
1,3,5-trinitrobenzene	99-35-4	213.1044	1.01	-3.31	-8.82	-9.24
1,3-butadiene	106-99-0	54.0902	1.85	-1.97	0.27	-1.54
1,3-dinitrobenzene	99-65-0	168.1068	1	-2.98	-6.13	-6.98
1,4-diamino-2,3-dihydroanthraquinone (DDA) violet-dye mix	81-63-0	240.2568	2.75	-3.31	-15.2	-15.65
1,4-di-p-toluidinoanthraquinone (PTA) solvent green 3	128-80-3	418.4856	6.72	-5.93	-18.28	-11.44
1-butanol	71-36-3	74.1212	0.9	-0.31	-1.84	-4.71
1-butene	106-98-9	56.106	2.08	-2.25	0.4	-0.65
1-chloro-2-methylbenzene	95-49-8	126.5829	3.18	-3.07	-2.29	-2.54
1-chloro-3-methylbenzene	108-41-8	126.5829	3.18	-3.07	-2.27	-2.48
1-hexene	592-41-6	84.159	3.05	-2.76	--[1]	--[1]
1-pentene	109-67-1	70.1325	2.57	-2.48	-0.11	-0.53
1-(methylamino)anthraquinone (disperse red 9)	82-38-2	237.2529	3.84	-4.03	-10.13	-9.15
2-(2-quinolyl)-1,3-indandione (D & C yellow no. 11) or (solvent yellow 33)	8003-22-3	273.285	3.01	-4.03	--[1]	--[1]
2,3-butanedione	431-03-8	86.089	0.13	0.34	-1.64	-5.89
2,3,7,8-tetrachlorodibenzo-p-dioxin	1746-01-6	321.9696	6.24	-8.29	-11.62	-4.85
2-methyl-1,3,5-trinitrobenzene	118-96-7	227.1309	1.21	-3.49	-8.75	-8.56
1-methyl-2,4-dinitrobenzene	121-14-2	182.1333	1.41	-3.19	-6.27	-6.58
2-methyl-1,3-dinitrobenzene	606-20-2	182.1333	1.41	-3.08	-6.26	-6.27
2,5-dimethylfuran	625-86-5	96.1268	2.17	-0.55	-1.08	-2.39
2-methyl-3,5-dinitrobenzenamine	35572-78-2	197.1479	1.25	-2.59	--[1]	--[1]
2-amino-9,10-anthracenedione (a) (AAQ)	117-79-3	223.2264	2.79	-4.07	-13.03	-10.72
2-butanone	78-93-3	72.1054	0.61	0.26	-0.88	-4.13
2-furaldehyde	98-01-1	96.0839	0.7	-0.8	-2.12	-5.18
2-heptanone	110-43-0	114.1849	2.06	-1.62	-2.15	-3.92
2-methyl-1-butene	563-46-2	70.1325	2.31	-2.47	-0.09	-0.63
2-methylfuran	534-22-5	82.1003	1.76	-0.56	-0.48	-2.29
2-methylthiophene	554-14-3	98.1669	2.28	-1.82	-1.4	-2.6
1-methyl-2-nitrobenzene	88-72-2	137.1357	1.88	-2.71	-3.64	-4.38
2-pentanone	107-87-9	86.1319	1.09	-0.29	-1.25	-4.05
isopropyl alcohol	67-63-0	60.0947	0.19	0.65	-1.21	-4.68

(Sheet 1 of 5)

[1] Not determined.

Table 4 (Continued)

Compound	CAS Number	MW g/mole	LogP (K_{ow}) Log()	Solubility Log(mg/mL)	Vapor Pressure Log(atm)	Henry's Law Log(atm/(mol/m^3))
2-thiophenecarboxaldehyde	98-03-3	112.1505	1.27	-1.53	-2.85	-5.41
3-(phenylhydrazone)-1H-indole-2,3-d	17310-26-8	237.2562	3.12	-3.7	-11.86	-9.65
3-furaldehyde	498-60-2	96.0839	0.69	-0.69	-1.98	-5.09
3-methyl-1-butene	563-45-1	70.1325	2.33	-2.42	0.05	-0.39
3-methylfuran	930-27-8	82.1003	1.76	-0.35	-0.56	-2.38
3-methylthiophene	616-44-4	98.1669	2.28	-1.66	-1.5	-2.69
1-methyl-3-nitrobenzene	99-08-1	137.1357	1.88	-2.73	-3.81	-4.82
4-amino-2,6-dinitrobenzene	19406-51-0	197.1479	1.97	-2.96	--[1]	--[1]
4-ethyltoluene	622-96-8	120.1911	3.51	-3.43	-2.37	-2.21
methyl isobutyl ketone	108-10-1	100.1584	1.35	-0.74	-1.54	-3.91
1-methyl-4-nitrobenzene	99-99-0	137.1357	1.88	-2.73	-4.06	-4.86
4-phenoxy-2(1H)-quinolinone	66662-28-0	237.2529	3.09	-4.02	-9.97	-8.88
acenaphthene	83-32-9	154.2074	4.16	-4.88	--[1]	--[1]
acenaphthylene	208-96-8	152.1916	4.13	-5.01	-5.16	-4.32
acetaldehyde	75-07-0	44.0524	-0.41	0.42	-0.17	-4.06
acetic acid	64-19-7	60.0518	-0.39	1.03	-1.56	-6.7
acetone	67-64-1	58.0789	0.12	0.43	-0.52	-4.14
acetonitrile	75-05-8	41.0518	-0.33	0.41	-1	-4.81
acetophenone	98-86-2	120.1482	1.67	-1.67	-3.37	-5.27
acetylene	74-86-2	26.0372	0.14	-0.02	1.8	-1.22
acrolein	107-02-8	56.0631	0.33	-0.25	-0.34	-3.65
acrylonitrile	107-13-1	53.0625	0.35	0.02	-0.13	-3.68
aluminum	7429-90-5	26.98154	--[2]	--[2]	--[2]	--[2]
anthracene	120-12-7	178.2288	4.71	-5.68	--[1]	--[1]
antimony	7440-36-0	121.75	--[2]	--[2]	--[2]	--[2]
arsenic	7440-38-2	74.92159	--[2]	--[2]	--[2]	--[2]
barium	7440-39-3	137.327	--[2]	--[2]	--[2]	--[2]
benzaldehyde	100-52-7	106.1217	1.52	-1.9	-2.69	-4.79
7h-benz[de]anthracen-7-one	82-05-3	230.2603	3.86	-5.88	-10.13	-6.68
benzene	71-43-2	78.1116	2.21	-2.39	-0.87	-2.37
benz[a]anthracene	56-55-3	228.2874	5.96	-7.02	--[1]	--[1]
benzo[a]pyrene	50-32-8	252.3088	6.62	-7.89	--[1]	--[1]
benz[e]acephenanthrylene	205-99-2	252.3088	6.32	-7.73	-11.16	-6.04
benzo(e)pyrene	192-97-2	252.3088	6.62	-7.89	-11.16	-5.94
benzo[ghi]perylene	191-24-2	276.3302	7.29	-9.22	-12.86	-6.29
benzo[k]fluoranthene	207-08-9	252.3088	6.32	-7.73	-11.73	-6.14
benzofuran	271-89-6	118.1324	2.6	-2.83	-2.48	-3.27
benzonitrile	100-47-0	103.1211	1.66	-1.83	-2.78	-4.99
beryllium	7440-41-7	9.0122	--[2]	--[2]	--[2]	--[2]

(Sheet 2 of 5)

[1] Not determined.
[2] Not applicable.

Table 4 (Continued)

Compound	CAS Number	MW g/mole	LogP (K_{ow}) Log()	Solubility Log(mg/mL)	Vapor Pressure Log(atm)	Henry's Law Log(atm/(mol/m^3))
bis(2-ethylhexyl)phthalate	117-81-7	390.5546	7.91	-6.23	-10.98	-5.37
butanal	123-72-8	72.1054	0.56	-0.53	-0.93	-3.98
cadmium	7440-43-9	112.411	--[2]	--[2]	--[2]	--[2]
calcium	7440-70-2	40.078	--[2]	--[1]	--[2]	--[2]
carbon dioxide (CO2)	124-38-9	44.0095	0.03	0.88	--[1]	--[1]
carbon disulfide	75-15-0	76.1427	1.4	-2.72	--[1]	--[1]
carbon monoxide (CO)	630-08-0	28.0104	-0.68	0.3	--[1]	--[1]
carbontetrachloride	56-23-5	153.8215	2.6	-2.72	-0.78	-1.96
carbonyl sulfide	463-58-1	60.0761	0.72	-1.38	--[1]	--[1]
chlorobenzene	108-90-7	112.5564	2.77	-2.88	-1.72	-2.48
chloroethene (vinyl chloride)	75-01-4	62.4978	1.69	-1.45	0.58	-1.42
chloroform	67-66-3	119.3767	1.74	-2.08	-0.68	-2.68
chloromethane	74-87-3	50.4871	0.98	-0.57	0.8	-1.86
chromium	7440-47-3	51.9961	--[2]	--[2]	--[2]	--[2]
chrysene	218-01-9	228.2874	5.96	-7.02	--[1]	--[1]
cis-2-butene	590-18-1	56.106	2.11	-1.79	0.35	-0.8
chlorine	7782-50-5	70.9054	1.2	-1.04	0.65	-1.23
cobalt	7440-48-4	58.9332	--[2]	--[2]	--[2]	--[2]
copper	7440-50-8	63.546	--[2]	--[2]	--[2]	--[2]
dibenz[a,h]anthracene	53-70-3	278.346	7.21	-7.92	-13.46	-6.62
dibenzo(b,def)chrysene-7,14-dione	128-66-5	332.3504	4.51	-7.32	-17.19	-9.81
dibutyl phthalate	84-74-2	278.3426	4.49	-4.07	-7.77	-5.79
dichloroacetonitrile	3018-12-0	109.9414	0.99	-1.04	-1.9	-4.91
dichlorodifluoromethane	75-71-8	120.9129	1.95	-2.24	0.77	-0.64
dimethyl trisulfide	3658-80-8	126.2668	1.57	-2.36	-3.07	-4.07
diphenylamine	122-39-4	169.222	3.3	-3.15	-5.53	-5.31
ethane	74-84-0	30.0688	1.34	-0.75	1.52	-0.12
ethanol	64-17-5	46.0682	-0.07	1.14	-1.06	-5.01
ethyl benzene	100-41-4	106.1646	3.1	-2.92	-1.8	-2.21
ethyl chloride	75-00-3	64.5136	1.46	-1.19	0.19	-1.94
ethylene	74-85-1	28.053	1.08	-0.69	1.76	-0.6
fluoranthene	206-44-0	202.2502	5.07	-6.74	--[1]	--[1]
fluorene	86-73-7	166.2181	4.21	-5.14	--[1]	--[1]
formaldehyde	50-00-0	30.0259	-0.68	0.3	0.82	-3.41
furan	110-00-9	68.0738	1.35	-0.88	0.05	-2.23
HCl	7647-01-0	36.4606	0.22	-1.04	--[1]	--[1]
heptanal	111-71-7	114.1849	2.02	-1.73	-2.15	-3.51
hexachlorobenzene	118-74-1	284.7804	4.9	-5.53	-7.38	-2.89
hexachlorobutadiene	87-68-3	260.759	4.78	-3.8	-4.01	-2.19

(Sheet 3 of 5)

[1] Not determined.
[2] Not applicable.

Table 4 (Continued)

Compound	CAS Number	MW g/mole	LogP (K_{ow}) Log()	Solubility Log(mg/mL)	Vapor Pressure Log(atm)	Henry's Law Log(atm/(mol/m^3))
hexachlorocyclopentadiene	77-47-4	272.7697	5.04	-4.28	-3.49	-3.05
hexachloroethane	67-72-1	236.7376	4.27	-3.69	-4	-2.74
hexanal	66-25-1	100.1584	1.53	-1.65	-1.74	-3.71
hexane	110-54-3	86.1748	3.28	-3.11	-0.65	0.12
octahydro-1,3,5,7-tetranitro-1,3,5,	2691-41-0	296.1548	-2.66	-2.22	-16.37	-14.56
hydrogen cyanide (hydrocyanic acid)	74-90-8	27.0253	-0.69	0.76	2.17	-1.54
isobutane	75-28-5	58.1218	2.08	-1.87	0.55	0.18
2-methyl-1-propene	115-11-7	56.106	1.83	-1.73	0.43	-0.67
indeno[1,2,3-cd]pyrene	193-39-5	276.3302	6.98	-8.17	-11.9	-6.25
isothiocyanatomethane	556-61-6	73.1178	1.46	-1.02	--[1]	--[1]
lead	7439-92-1	207.19	--[2]	--[2]	--[2]	--[2]
xylene (mixed isomers)	1330-20-7	106.1646	--[1]	--[1]	--[1]	--[1]
1,3-dimethylbenzene	108-38-3	106.1646	3.03	-3.17	-1.91	-2.31
p-xylene	106-42-3	106.1646	3.03	-3.17	-1.95	-2.31
magnesium	7439-95-4	24.305	--[2]	--[1]	--[2]	--[2]
manganese	7439-96-5	54.938	--[2]	--[1]	--[2]	--[2]
1,3-dichlorobenzene	541-73-1	147.0012	3.34	-3.34	-2.39	-2.57
mercury	7439-97-6	200.59	--[2]	--[1]	-5.6	--[2]
methacrolein	78-85-3	70.0896	0.57	-0.54	-0.7	-3.52
methane	74-82-8	16.0423	0.45	-1.1	2.17	-0.06
methylene chloride	75-09-2	84.9319	1.35	-1.41	-0.27	-2.74
methyl nitrite	624-91-9	61.0399	-0.36	-0.68	-0.5	-4.79
2-methoxy-2-methylpropane (MTBE)	1634-04-4	88.1477	1.36	-0.05	-0.25	-2.49
3-buten-2-one	78-94-4	70.0896	0.27	-0.01	-1.01	-4.04
naphthalene	91-20-3	128.1702	3.46	-4.16	--[1]	--[1]
butane	106-97-8	58.1218	2.31	-2.32	0.39	-0.06
decane	124-18-5	142.2808	5.22	-5.14	-2.72	0.68
ammonia	7664-41-7	17.0304	-1.24	-1.04	--[1]	--[1]
nickel	7440-02-0	58.69	--[2]	--[2]	--[2]	--[2]
nitric acid	7697-37-2	63.0128	-0.55	-1.04	-5.25	-9.36
nitrobenzene	98-95-3	123.1092	1.47	-2.27	-3.39	-4.87
nitrogen dioxide	10102-44-0	46.0055	-2.04	-1.04	--[1]	--[1]
nitroglycerin	55-63-0	227.0863	-2.47	-3.08	-6.7	-7.55
nitromethane	75-52-5	61.0399	-0.59	-0.17	--[1]	--[1]
nonanal	124-19-6	142.2379	2.99	-3.44	-3.24	-3.32
octachlorodibenzo[b,e][1,4]dioxin	3268-87-9	459.7488	8.44	-9.88	-15.08	-4.92
octanal	124-13-0	128.2114	2.5	-2.39	-2.62	-3.42
o-dichlorobenzene	95-50-1	147.0012	3.31	-3.43	-2.65	-2.76
o-methoxy-phenyl-azo-b-naphtho	1229-55-6	278.3047	5.13	-5.67	-13.3	-10.4

(Sheet 4 of 5)

[1] Not determined.
[2] Not applicable.

Table 4 (Concluded)

Compound	CAS Number	MW g/mole	LogP (K_{ow}) Log()	Solubility Log(mg/mL)	Vapor Pressure Log(atm)	Henry's Law Log(atm/(mol/m^3))
1,2-dimethylbenzene (o-xylene)	95-47-6	106.1646	3.03	-3.17	--[1]	--[1]
NaCN, particulate cyanide	57-12-5	49.0072	-0.69	-1.04	--[1]	--[1]
p-dichlorobenzene	106-46-7	147.0012	3.18	-3.31	-2.71	-2.63
pentaerythritol tetranitrate	78-11-5	316.1363	-3.17	-3.9	-7.55	-7.12
perchloroethylene	127-18-4	165.8322	3.24	-2.44	-1.29	-1.18
phenanthrene	85-01-8	178.2288	4.71	-5.68	--[1]	--[1]
phenol	108-95-2	94.111	1.59	-0.32	-3.38	-6.18
phenylethyne	536-74-3	102.133	2.31	-2.74	-1.63	-2.37
phosphorus	7723-14-0	30.9738	--[2]	--[1]	--[2]	--[2]
propanal	123-38-6	58.0789	0.08	0.34	-0.55	-4
propane	74-98-6	44.0953	1.83	-1.5	0.96	0.02
propene	115-07-1	42.0795	1.59	-1.47	0.97	-0.55
1-propyne	74-99-7	40.0637	1.03	-1.08	0.73	-1.82
pyrene	129-00-0	202.2502	5.37	-6.72	--[1]	--[1]
hexahydro-1,3,5-trinitro-1,3,5-tria	121-82-4	222.1161	-1.89	-2	-11.88	-11.37
selenium	7782-49-2	78.96	--[2]	--[1]	--[2]	--[2]
silver	7440-22-4	107.8682	--[2]	--[2]	--[2]	--[2]
styrene	100-42-5	104.1488	2.87	-2.73	--[1]	--[1]
sulfur dioxide (7446-09-5)	7446-09-5	64.0648	-1.45	-0.84	--[1]	--[1]
sulfuric acid	7664-93-9	98.0794	-1.84	-1.04	-9.97	-14.3
n-methyl-n,2,4,6-tetranitroaniline	479-45-8	287.1431	0.92	-4.44	-0.88	-8.27
thallium	7440-28-0	204.3833	--[2]	--[2]	--[2]	--[2]
thiophene	110-02-1	84.1404	1.87	-2	-0.93	-2.68
toluene	108-88-3	92.1381	2.62	-2.67	--[1]	--[1]
(E)-2-butenal	123-73-9	70.0896	0.85	-0.36	-0.74	-3.57
(E)-2-butene	624-64-6	56.106	2.11	-1.79	0.35	-0.8
(E)-2-pentene	646-04-8	70.1325	2.59	-2.01	-0.14	-0.66
3-penten-2-one	625-33-2	84.1161	0.78	-0.17	-1.4	-3.98
trichloroethylene	79-01-6	131.3874	2.76	-2.15	-0.75	-1.59
trichloroflouromethane	75-69-4	137.3672	2.24	-2.39	0.09	-1.24
vinylidenechloride	75-35-4	96.9426	2.24	-1.78	0.15	-0.94
zinc	7440-66-6	65.39	--[2]	--[2]	--[2]	--[2]

(Sheet 5 of 5)

[1] Not determined.
[2] Not applicable.

Data gaps

For the compounds that had property values that could not be calculated or estimated by the means employed in this study, it would be extremely useful to extend the estimation tools to be able to include these compounds. The prediction/estimation of the HLC is the area that would require the most

development work as no working training set existed for the use of QSAR/QSPR techniques. It was also clear that the HLC training set will need to be significant in size (greater than a few thousand compounds) as the training done with the approximately hundred values was not even successful in reliably predicting back onto itself (common method to evaluate the quality of the training set being used). The other parameters (besides HLC) predicted for organic compounds were quite successful; however, the models were not readily applicable to inorganic compounds. The difficulty with predicting properties with the majority of inorganics is twofold. First, the inorganics, while often containing covalent components, are most often highly polar or ionic in nature, which meant that the organic type models could not be applied. Second, many of the inorganics (particularly the metals) will form numerous species (e.g. different oxidation states and coordination compounds), each of which will need to be individually identified and then evaluated to predict its properties in solution. Therefore, it is recommended that further work on the inorganic species and selected organic compounds with the development of fully optimized QSPR/QSAR tools be considered.

Diffusion Coefficients

Methods

Diffusion coefficients were not included in the list of parameters in the initial study (Zakikhani et al. 2002). The diffusion coefficients have been added as additional fate and transport properties for chemicals in water and air. Diffusion is the transport of molecules in a liquid or gas medium due to the intermolecular collisions rather than turbulence or transport. This process is promoted by gradients, such as pressure, temperature, and concentration. A number of diffusion coefficients were found in the literature. When diffusion coefficients could not be located for a constituent, the values were calculated using the following methods. Each of these methods was applied assuming an ambient temperature of 25 °C and a pressure of 1 atm.

Hayduk and Laudie. [Hayduk and Laudie (1974).] This method is used to calculate the diffusion coefficient for organic constituents in water. It is comparable to the Wilke-Chang and Scheibel methods in terms of input parameters, accuracy, and general applicability but has been recommended by Reid et al. (1977) because the computation is easier than the previously mentioned methods, and it has been validated by a more recently compiled database. According to Lyman et al. (1982a), the Hayduk and Laudie method produced results for 87 solutes with an absolute average error of 5.8 percent. This method is given by the following equation:

$$D_{BW} = \frac{13.26 \times 10^{-5}}{\eta_w^{1.14} V_B'^{0.589}} \quad (6)$$

where

D_{BW} = Diffusion coefficient of solute *B* into water (cm^2/sec)

η_w = Viscosity of water (cP)

V'_B = LeBas molar volume of solute *B* (cm^3/g-mole)

Fuller, Schettler, and Giddings (FSG). [Fuller et al. (1966).] This method is used to predict binary gas phase diffusivities. It is most accurate for nonpolar gases at low to moderate temperatures and least accurate for polar acids and glycols. Lyman et al. (1982a) reports the best results with this method are obtained for halogenated hydrocarbons with an absolute average error of 1.7 percent for 22 compounds that were tested. The worst results reported by Lyman et al. (1982a) were for acids with an absolute average error of 12.4 percent for 8 compounds that were tested. This method is described using the following equation:

$$D_{BA} = \frac{10^{-3} T^{1.75} \sqrt{M_r}}{P\left(V_A^{1/3} + V_B^{1/3}\right)^2} \tag{7}$$

where

D_{BA} = Diffusion coefficient of gas *B* into air (cm^2/sec)

T = Temperature (°K)

M_r = $(M_A + M_B) / M_A M_B$

M_A = Molecular weight of air (g/g-mole)

M_B = Molecular weight of gas *B* (g/g-mole)

P = Pressure (atm)

V_A = Molar volume of air (cm^3/g-mole)

V_B = Molar volume of gas *B* (cm^3/g-mole)

Wilke-Lee. [Wilke and Lee (1955).] This method is used to calculate the diffusion coefficient for gases and vapors in a binary gas phase system. It is reported to be usable for a wider range of compounds and temperatures than is the FSG method. Jarvis and Lugg (1968) and Lugg (1968) reported an absolute average error of 4.3 percent for 150 compounds tested, and all classes of compounds examined had average errors of less than 8 percent with the exception of acids. This method is outlined below:

$$D_{BA} = \frac{B' T^{3/2} \sqrt{M_r}}{P \sigma_{AB}^2 \Omega} \tag{8}$$

where

D_{BA} = Diffusion coefficient of gas *B* into air (cm^2/sec)

$$B' = 0.00217 - 0.00050 \sqrt{\frac{1}{M_A} + \frac{1}{M_B}}$$

T = Temperature (°K)

M_r = $(M_A + M_B) / M_A M_B$

M_A = Molecular weight of air (g/g-mole)

M_B = Molecular weight of gas *B* (g/g-mole)

P = Pressure (atm)

The collision integral, Ω, is a function of the molecular energy of attraction, ϵ, and the Boltzmann constant, *k*, as shown below.

$$\Omega = \frac{s}{(T^*)^t} + \frac{u}{e^{T^* v}} + \frac{w}{e^{T^* x}} + \frac{y}{e^{T^* z}} \tag{9}$$

where

$s = 1.06036$	$u = 0.19300$	$w = 1.03587$	$y = 1.76474$
$t = 0.15610$	$v = 0.47635$	$x = 1.52996$	$z = 3.89411$

and

$$T^* = \frac{T}{(\varepsilon / k)_{AB}} \tag{10}$$

$$(\varepsilon / k)_{AB} = \sqrt{(\varepsilon / k)_A (\varepsilon / k)_B} \tag{11}$$

where $(\varepsilon / k)_A = 78.6K$ and $(\varepsilon / k)_B = 1.15 T_b(K)$.

The characteristic length, σ_{AB}, is a function of the molal volume at the boiling point, V_B' :

$$\sigma_{AB} = \frac{\sigma_A + \sigma_B}{2} \tag{12}$$

where $\sigma_A = 3.711$ Å and $\sigma_B = 1.18(V_B')^{1/3}$.

USEPA (1994). The USEPA recommends correlations for estimating gas phase and liquid phase diffusion coefficients in the documentation for the WATER9 Wastewater Treatment Model. These are simplified calculations that involve the temperature, molecular weight, and density of the constituent and are used in situations when limited resources preclude the use of more complex correlations or when limited constituent data are available. According to the documentation, the estimated median error of the vapor phase diffusion coefficient is 7 percent. These correlations are given by the following equations:

$$D_v = \frac{0.00229\left(T + 273.16\right)^{1.5}\sqrt{0.034 + \frac{1}{Mwt}}\left(1 - 0.000015Mwt^2\right)}{\left[\left(\frac{Mwt}{2.5\rho}\right)^{0.333} + 1.8\right]^2} \tag{13}$$

where

D_v = Gas phase diffusion constant (cm^2/sec)

T = Temperature (°C)

Mwt = Molecular weight of the gas (g/g-mole)

ρ = Density (g/cc)

$$D_l = 0.0001518\left(\frac{T + 273.16}{298.16}\right)\left(\frac{Mwt}{\rho}\right)^{-0.6} \tag{14}$$

where

D_l = Liquid phase diffusion constant (cm^2/sec)

T = Temperature (°C)

Mwt = Molecular weight of the compound (g/g-mole)

ρ = Pure compound liquid density (g/cc)

Analysis

Literature values for the diffusion coefficient in air were found for 35 of the 188 chemicals. For the diffusion coefficient in water, a total of 90 values were found. This provided a set of data with which the calculated values could be compared. Table 5 shows all of the values found during the literature search for the diffusion coefficient in air (*Da*) and the diffusion coefficient in water (*Dw*) with the reference number for each one in parentheses; the full references are cited below the table. Any literature values known to be calculated or estimated were not included or used for validation of the methods listed above.

Table 5
Literature Values for Diffusion Coefficients

ID	Chemical	CAS Number	*Da*, cm^2/sec	*Dw*, cm^2/sec
1	1,2-dichloroethene (cis)	156-59-2		
2	1,2-dichloroethene (trans)	156-60-5		1.03E-5 (5)
3	(1,2-dichloroethyl) benzene	1074-11-9		
4	1,2,4-trimethylbenzene	95-63-6		
5	1,2-dichlorethane	107-06-2		1.01E-5 (5)
6	1,2-dichloro-3-methylbenzene	32768-54-0		
7	1,2-dichloroethene (cis/trans mixture)	540-59-0		
8	1,3,5-trimethylbenzene (mesitylene)	108-67-8		
9	1,3,5-trinitrobenzene	99-35-4		
10	1,3-butadiene	106-99-0		9.5E-6 (5)
11	1,3-dinitrobenzene	99-65-0		
12	1,4-diamino-2,3-dihydroanthraquinone (DDA) violet-dye mix	81-63-0		
13	1,4-di-p-toluidinoanthraquinone (PTA) solvent green 3	128-80-3		
14	1-butanol	71-36-3	7.27E-2 (6)	9.7E-6 (5)
15	1-butene	106-98-9		
16	1-chloro-2-methylbenzene	95-49-8		
17	1-chloro-3-methylbenzene	108-41-8	5.4E-2 (6)	
18	1-hexene	592-41-6	7.19E-2 (9)	
19	1-pentene	109-67-1	8.29E-2 (9)	
20	1-(methylamino)anthraquinone (disperse red 9)	82-38-2		
21	2-(2-quinolyl)-1,3-indandione (D & C yellow no. 11) or (solvent yellow 33)	8003-22-3		
22	2,3-butanedione	431-03-8		
23	2,3,7,8-tetrachlorodibenzo-p-dioxin	1746-01-6		

(Sheet 1 of 5)

1. USEPA (1996). "Soil screening guidance: Technical background document," EPA/540/R95/128, Office of Emergency and Remedial Response, Washington, DC. (NTIS PB96-963502.)
2. USEPA (1994). "Air emissions models for waste and wastewater, WATER9," http://www.epa.gov/ttn/chief/software/water/.
3. USEPA Region IX Preliminary Remediation Goals. http://www.epa.gov/region09/waste/sfund/prg/index.html
4. Oak Ridge National Laboratories, Risk Assessment Information System. (2005). http://risk.lsd.ornl.gov/rap_hp.shtml
5. Montgomery. (1996). *Groundwater chemicals desk reference*. 2nd ed., Lewis Publishers.
6. Perry et al. (1997). *Perry's chemical engineer's handbook*. 7th ed., McGraw-Hill, New York.
7. Gustafson et al. (1997). "Selection of Representative TPH Fractions Based on Fate and Transport Considerations," TPH Working Group Series on-line, Volume 3, http://www.aehs.com/publications/catalog/contents/tph.htm
8. Lide (1997). *CRC handbook of chemistry and physics*. 78th ed., CRC Press.
9. Lyman et al. (1992). "Contaminants dissolved in groundwater." *Mobility and degradation of organic contaminants in subsurface environments*. C.K. Smoley, Inc., Chelsea, MI, 207-235.
10. Thibodeaux (1995). Environmental chemodynamics: Movement of chemicals in air, water, and soil. 2nd ed.
11. Li and Gregory (1974). "Diffusion of ions in sea water and in deep-sea sediments," *Geochemicha et Cosmochimica Acta* 38, 703-714.
12. USEPA (1995e). "OAQPS," Emission Factor and Inventory Group, Air Emission Models Wastewater Treatment, Version 4.0, Research Triangle Park, NC.

Table 5 (Continued)

ID	Chemical	CAS Number	*Da*, cm^2/sec	*Dw*, cm^2/sec
24	2,4,6-trinitrotoluene (TNT)	118-96-7		
25	2,4-dinitrotoluene (DNT; 2,4-DNT)	121-14-2		
26	2,6-dinitrotoluene (2,6-DNT)	606-20-2		7.6E-6 (1,2,4,5)
27	2,5-dimethylfuran	625-86-5		
28	2-amino-4,6-dinitrotoluene	35572-78-2		
29	2-amino-9,10-anthracenedione (a) (AAQ)	117-79-3		
30	2-butanone	78-93-3		9.4E-6 (5)
31	2-furaldehyde	98-01-1		1.12E-5 (5)
32	2-heptanone	110-43-0		
33	2-methyl-1-butene	563-46-2		
34	2-methylfuran	534-22-5		
35	2-methylthiophene	554-14-3		
36	2-nitrotoluene (ONT)	88-72-2		
37	2-pentanone	107-87-9		8.5E-6 (5)
38	2-propanol	67-63-0	1.01E-1 (10)	
39	2-thiophenecarboxaldehyde	98-03-3		
40	3-(phenylhydrazone)-1H-indole-2,3-dione	17310-26-8		
41	3-furaldehyde	498-60-2		
42	3-methyl-1-butene	563-45-1		
43	3-methylfuran	930-27-8		
44	3-methylthiophene	616-44-4		
45	3-nitrotoluene	99-08-1		
46	4-1,2,4-oxadizaolin-3-one-2,5-diphenyl-delta	Unknown		
47	4-amino-2,6-dinitrotoluene (4ADNT)	19406-51-0		
48	4-ethyltoluene	622-96-8		
49	4-methyl-2-pentanone	108-10-1		7.7E-6 (5)
50	4-nitrotoluene	99-99-0		
51	4-phenoxy-2(1H)-quinolinone	66662-28-0		
52	acenaphthene	83-32-9		6.4E-6 (5)
53	acenaphthylene	208-96-8		
54	acetaldehyde	75-07-0		
55	acetic acid	64-19-7	1.33E-1 (10)	1.24E-5 (6)
56	acetone	67-64-1	1.09E-1 (10)	1.28E-5 (5,8)
57	acetonitrile	75-05-8		1.23E-5 (5)
58	acetophenone	98-86-2		
59	acetylene	74-86-2		2.11E-5 (6)
60	acrolein	107-02-8		1.12E-5 (5)
61	acrylonitrile	107-13-1		1.12E-5 (5)
62	aluminum	7429-90-5		5.59E-6 (11)
63	anthracene^{3+}	120-12-7	4.21E-2 (10)	5.9E-6 (5)
64	antimony	7440-36-0		8.25E-6 (10)
65	arsenic	7440-38-2		9.05E-6 (10)
66	barium^{2+}	7440-39-3		8.48E-6 (11)
67	benzaldehyde	100-52-7		
68	benzanthrone (b)	82-05-3		
69	benzene	71-43-2	8.8E-2 (10)	1.09E-5 (5)
70	benzo(a)anthracene	56-55-3		5.2E-6 (5)
71	benzo(a)pyrene	50-32-8		5E-6 (5)
72	benzo(b)fluoranthene	205-99-2		4.9E-6 (5)
73	benzo(e)pyrene	192-97-2		
74	benzo(g,h,i)perylene	191-24-2		4.9E-6 (5)
75	benzo(k)fluoranthene	207-08-9		4.9E-6 (5)

(Sheet 2 of 5)

Table 5 (Continued)

ID	Chemical	CAS Number	*Da*, cm^2/sec	*Dw*, cm^2/sec
76	benzofuran	271-89-6		
77	benzonitrile	100-47-0		
78	beryllium^{2+}	7440-41-7		5.85E-6 (11)
79	bis(2-ethylhexyl)phthalate	117-81-7		3.9E-6 (5)
80	butanal	123-72-8		
81	cadmium^{2+}	7440-43-9		7.17E-6 (10)
82	calcium^{2+}	7440-70-2		7.93E-6 (10)
83	carbon dioxide (CO2)	124-38-9	1.64E-1 (10)	1.77E-5 (10)
84	carbon disulfide	75-15-0	1.07E-1 (10)	
85	carbon monoxide (CO)	630-08-0	2.03E-1 (10)	2.17E-5 (10)
86	carbon tetrachloride	56-23-5	8.28E-2 (10)	8.8E-6 (1,2,3,4,5)
87	carbonyl sulfide	463-58-1		
88	chlorobenzene	108-90-7	6.2E-2 (10)	8.7E-6 (1,2,3,4,5)
89	chloroethene (vinyl chloride)	75-01-4		
90	chloroform	67-66-3	9.1E-2 (10)	1E-5 (1,3,4,5)
91	chloromethane	74-87-3	9.1E-2 (10)	1.49E-5 (5)
92	chromium^{3+}	7440-47-3		5.94E-6 (10)
93	chrysene	218-01-9		6.3E-6 (5)
94	cis-2-butene	590-18-1		
95	Cl2 (a)	7782-50-5	9.3E-2 (10)	1.44E-5 (6)
96	cobalt^{2+}	7440-48-4		1.12E-5 (10)
97	copper^{2+}	7440-50-8		7.33E-6 (10)
98	dibenz(a,h)anthracene	53-70-3		4.6E-6 (5)
99	dibenzo(b,def)chrysene-7,14 dione (c.i. vat yellow 4)	128-66-5		
100	dibutyl phthalate	84-74-2		4.9E-6 (5)
101	dichloroacetonitrile	3018-12-0		
102	dichlorodiflouromethane	75-71-8		9.3E-6 (5)
103	dimethyltrisulfide	3658-80-8		
104	diphenylamine	122-39-4		
105	ethane	74-84-0	1.08E-1 (10)	
106	ethanol	64-17-5	1.19E-1 (10)	1.24E-5 (8)
107	ethyl benzene	100-41-4	7.7E-2 (10)	8.1E-6 (5)
108	ethyl chloride	75-00-3		1.07E-5 (5)
109	ethylene	74-85-1		
110	fluoranthene	206-44-0		5.6E-6 (5)
111	fluorene	86-73-7		6.1E-6 (5)
112	formaldehyde	50-00-0		
113	furan	110-00-9		
114	HCl	7647-01-0	1.73E-1 (10)	3.1E-5 (6)
115	heptanal	111-71-7		
116	hexachlorobenzene	118-74-1		5.5E-6 (5)
117	hexachlorobutadiene	87-68-3		6.5E-6 (5)
118	hexachlorocyclopentadiene	77-47-4		6.7E-6 (5)
119	hexachloroethane	67-72-1		6.3E-6 (5)
120	hexanal	66-25-1		
121	hexane	110-54-3	8E-2 (10)	
122	HMX	2691-41-0		
123	hydrogen cyanide	74-90-8	1.73E-1 (10)	1.82E-5 (3)
124	i-butane (isobutane)	75-28-5	9.11E-2 (9)	
125	i-butene (isobutene/e-butylene)	115-11-7		
126	indeno(1,2,3-cd)pyrene	193-39-5		4.8E-6 (5)
127	isothiocyanatomethane	556-61-6		

(Sheet 3 of 5)

Table 5 (Continued)

ID	Chemical	CAS Number	*Da*, cm^2/sec	*Dw*, cm^2/sec
128	$lead^{2+}$	7439-92-1		9.45E-6 (10)
129	xylene (mixed isomers)	1330-20-7	7.1E-2 (10)	
130	m-xylene (meta-xylene)	108-38-3		7.8E-6 (1,2,3,4,5,7)
131	p-xylene (para-xylene)	106-42-3		7.9E-6 (5)
132	$magnesium^{2+}$	7439-95-4		7.05E-6 (11)
133	$manganese^{2+}$	7439-96-5		6.88E-6 (11)
134	m-dichlorobenzene	541-73-1		8.2E-6 (5)
135	mercury	7439-97-6	1.31E-1 (10)	2.9E-5 (10)
136	methacrolein	78-85-3		
137	methane	74-82-8	1.6E-1 (10)	1.49E-5 (8)
138	methylene chloride	75-09-2		1.15E-5 (5)
139	methylnitrite	624-91-9		
140	methyl-t-butylether (MTBE)	1634-04-4		
141	methyl-vinyl ketone	78-94-4		
142	naphthalene	91-20-3	5.13E-2 (10)	
143	n-butane	106-97-8		
144	n-decane	124-18-5		
145	NH3 (ammonia)	7664-41-7	2.8E-1 (10)	1.1E-5 (5)
146	$nickel^{2+}$	7440-02-0		6.79E-6 (11)
147	nitric acid	7697-37-2		2.98E-5 (6)
148	nitrobenzene	98-95-3		
149	nitrogen oxide (NOx)	10102-44-0	2.04E-1 (10)	2.55E-5 (10)
150	nitroglycerine	55-63-0		
151	nitromethane	75-52-5		
152	nonanal	124-19-6		
153	OCDD (1,2,3,4,6,7,8,9-OCDD)	3268-87-9		
154	octanal	124-13-0		
155	o-dichlorobenzene	95-50-1		8.2E-6 (5)
156	o-methoxy-phenyl-azo-b-naphthol (oil red g)	1229-55-6		
157	o-xylene (ortho-xylene)	95-47-6		7.9E-6 (5)
158	particulate cyanide	57-12-5	5.21E-1 (12)	2.28E-5 (12)
159	p-dichlorobenzene (para-dichlorobenzene)	106-46-7		8.2E-6 (5)
160	pentaerythritoltetranitrate (PETN)	78-11-5		
161	perchloroethylene	127-18-4		8.7E-6 (5)
162	phenanthrene	85-01-8		5.9E-6 (5)
163	phenol	108-95-2		8.7E-6 (5)
164	phenylacetylene (ethynyl benzene)	536-74-3		
165	phosphorus	7723-14-0		6.12E-6 (10)
166	propanal	123-38-6		
167	propane	74-98-6	8.8E-2 (10)	
168	propylene	115-07-1		
169	propyne	74-99-7		
170	pyrene	129-00-0		
171	RDX	121-82-4		
172	$selenium^{6+}$	7782-49-2		9.46E-6 (10)
173	$silver^{1+}$	7440-22-4		1.66E-7 (11)
174	styrene (vinyl benzene)	100-42-5		8.1E-6 (1,2,3,4,5,7)
175	sulfur dioxide (SO2)	7446-09-5	1.03E-1 (10)	1.7E-5 (6)
176	sulfuric acid	7664-93-9		1.97E-5 (6)
177	tetryl (2,4,6-trinitrophenylmethylnitramine)	479-45-8		6.4E-6 (5)
178	$thallium^{4+}$	7440-28-0		1.53E-6 (11)
179	thiophene	110-02-1		

(Sheet 4 of 5)

Table 5 (Concluded)

ID	Chemical	CAS Number	*Da*, cm^2/sec	*Dw*, cm^2/sec
180	toluene	108-88-3	8.8E-2 (10)	8.6E-6 (1,2,3,4,7,8)
181	trans-2-butenal	123-73-9		
182	trans-2-butene	624-64-6		
183	trans-2-pentene	646-04-8		
184	trans-3-penten-2-one	625-33-2		
185	trichloroethylene (TCE)	79-01-6		9.4E-6 (5)
186	trichloroflouromethane	75-69-4	9.02E-2 (10)	9.3E-6 (5)
187	vinylidenechloride	75-35-4		1.01E-5 (5)
188	$zinc^{2+}$	7440-66-6		7.15E-6 (10)

(Sheet 5 of 5)

The calculated values from each of the methods listed above were analyzed using the average model error (AME, Equation 5) and the average bias (Equation 4) discussed in Chapter 2. These statistical methods were used to examine the calculated values for the entire data set as well as for each individual class of chemicals to determine which methods gave the best overall results and the best results for each specific class.

The results of this analysis are shown in Tables 6 and 7 for the diffusion coefficient in air and water, respectively. The best methods for each class (group, see Table 1) of chemicals are noted in bold type. The overall results for each method are given in the last row of each table.

Table 6
Statistical Results for the Diffusion Coefficient in Air

	Estimation Technique					
	FSG		Wilke-Lee		EPA_{Air}	
Chemical Group	AME	Bias	AME	Bias	AME	Bias
alcohols/ketones	8.49	-2.38E-01	16.58	6.71E-01	**8.02**	**-9.46E-02**
biocides/dyes	**2.03**	**3.51E-01**	2.38	4.12E-01	3.03	-5.23E-01
explosives	-	-	-	-	-	-
furans+dioxins	-	-	-	-	-	-
gases	16.02	-2.38E-01	36.67	-1.40E+00	**15.47**	**-1.39E+00**
halogenated	**18.50**	**1.12E+00**	22.07	1.62E+00	26.02	-5.80E-01
hydrocarbons	**10.44**	**7.27E-01**	20.40	2.17E+00	19.65	-1.32E+00
hetals/inorganics	-	-	-	-	45.90	-6.01E+00
other	**4.08**	**-3.81E-01**	6.57	1.00E+00	7.97	-9.61E-01
PAHs+PCBs	35.32	1.64E+00	39.47	1.85E+00	**14.52**	**3.95E-01**
Overall	**13.42**	**4.13E-03**	23.26	9.77E-03	18.66	-1.07E-02

Table 7
Statistical Results for the Diffusion Coefficient in Water

Chemical Group	Estimation Technique			
	Hayduk-Laudie		EPA_{Water}	
	AME	Bias	AME	Bias
alcohols/ketones	6.84	3.63E-05	**6.48**	**2.00E-05**
biocides/dyes	-	-	-	-
explosives	**6.90**	**-4.72E-05**	-	-
furans+dioxins	-	-	-	-
gases	39.84	2.09E-06	**9.53**	**-2.37E-04**
halogenated	7.04	5.97E-05	**6.72**	**4.27E-05**
hydrocarbons	**9.23**	**6.57E-05**	9.72	-2.11E-05
metals/inorganics	-	-	**3.84**	**1.11E-04**
other	**37.43**	**-1.01E-03**	41.07	-1.27E-03
PAHs+PCBs	**12.86**	**6.23E-05**	-	-
Overall	12.46	3.89E-08	**8.26**	**-2.91E-07**

Results

The statistical analysis above shows that the diffusion coefficient in air and water can generally be predicted with an AME of less than 15 percent. Some classes of chemicals have higher AME values due to the nature of the chemicals in these classes. For instance, the "other" classification includes chemicals such as hydrochloric acid, sulfuric acid, and nitric acid. These chemicals are highly polar and dissociate rapidly in water. Lyman et al. (1982a) stated that the FSG and Wilke-Lee methods were both least accurate for acids, especially highly polar acids.

All values calculated with the methods listed at the beginning of this section are given in Table 8. If a field is empty, this signifies that there were insufficient data available for the constituent to calculate a value with the indicated method. The methods listed for the diffusion coefficient in air from left to right are FSG (Da_{FSG}), Wilke and Lee (Da_{WL}), and WATER9 (Da_{Water9}). The methods listed for the diffusion coefficient in water from left to right are Hayduk and Laudie (Dw_{HL}) and WATER9 (Dw_{Water9}).

Table 8
Calculated Values for Diffusion Coefficients

Chemical	CAS Number	Diffusion in Air			Diffusion in Water	
		Da_{FSG}	Da_{WL}	Da_{Water9}	Dw_{HL}	Dw_{Water9}
1,2-dichloroethene (cis)	156-59-2	9.09E-02	9.93E-02	8.62E-02	1.10E-05	1.11E-05
1,2-dichloroethene (trans)	156-60-5	9.09E-02	1.00E-01	8.54E-02	1.10E-05	1.10E-05
(1,2-dichloroethyl) benzene	1074-11-9	6.16E-02	6.38E-02		7.06E-06	
1,2,4-trimethylbenzene	95-63-6	6.62E-02	7.10E-02	5.92E-02	7.55E-06	7.79E-06
1,2-dichlorethane	107-06-2	8.89E-02	9.47E-02	8.33E-02	1.04E-05	1.08E-05
1,2-dichloro-3-methylbenzene	32768-54-0	6.57E-02	6.86E-02		7.62E-06	
1,2-dichloroethene (cis/trans mixture)	540-59-0	9.09E-02	9.96E-02		1.10E-05	

(Sheet 1 of 5)

Table 8 (Continued)

Chemical	CAS Number	Diffusion in Air			Diffusion in Water	
		Da_{FSG}	Da_{WL}	Da_{Water9}	Dw_{HL}	Dw_{Water9}
1,3,5-trimethylbenzene (mesitylene)	108-67-8	6.62E-02	7.12E-02	5.88E-02	7.55E-06	7.72E-06
1,3,5-trinitrobenzene	99-35-4	6.68E-02	6.11E-02	2.44E-02	7.07E-06	
1,3-butadiene	106-99-0	9.79E-02	1.14E-01	1.00E-01	1.13E-05	1.03E-05
1,3-dinitrobenzene	99-65-0	7.14E-02	6.73E-02	4.68E-02	7.82E-06	
1,4-diamino-2,3-dihydroanthraquinone (DDA) violet-dye mix	81-63-0	5.32E-02	5.10E-02		5.86E-06	
1,4-di-p-toluidinoanthraquinone (PTA) solvent green 3	128-80-3	3.80E-02	3.57E-02		4.09E-06	
1-butanol	71-36-3	8.73E-02	1.10E-01	8.78E-02	9.84E-06	9.93E-06
1-butene	106-98-9	9.53E-02	1.10E-01	9.52E-02	1.08E-05	9.74E-06
1-chloro-2-methylbenzene	95-49-8	7.09E-02	7.58E-02	6.13E-02	8.27E-06	8.57E-06
1-chloro-3-methylbenzene	108-41-8	7.09E-02	7.57E-02		8.27E-06	
1-hexene	592-41-6	7.57E-02	8.46E-02	7.33E-02	8.49E-06	8.24E-06
1-pentene	109-67-1	8.39E-02	9.52E-02	8.26E-02	9.45E-06	8.92E-06
1-(methylamino)anthraquinone (disperse red 9)	82-38-2	5.27E-02	5.18E-02		5.93E-06	
2-(2-quinolyl)-1,3-indandione (D & C yellow no. 11) or (solvent yellow 33)	8003-22-3	4.95E-02	4.75E-02		5.47E-06	
2,3-butanedione	431-03-8	8.65E-02	9.50E-02	8.30E-02	1.03E-05	1.01E-05
2,3,7,8-tetrachlorodibenzo-p-dioxin	1746-01-6	5.10E-02	5.00E-02		5.71E-06	
2,4,6-trinitrotoluene (TNT)	118-96-7	6.26E-02	5.97E-02	1.63E-02	6.61E-06	
2,4-dinitrotoluene (DNT; 2,4-DNT)	121-14-2	6.63E-02	6.30E-02	4.65E-02	7.22E-06	
2,6-dinitrotoluene (2,6-DNT)	606-20-2	6.63E-02	6.30E-02	5.42E-02	7.22E-06	
2,5-dimethylfuran	625-86-5	8.12E-02	8.73E-02		9.29E-06	
2-amino-4,6-dinitrotoluene	35572-78-2	6.44E-02	5.95E-02		6.90E-06	
2-amino-9,10-anthracenedione (a) (AAQ)	117-79-3	5.53E-02	5.11E-02		5.83E-06	
2-butanone	78-93-3	8.92E-02	1.23E-01	8.94E-02	1.03E-05	1.01E-05
2-furaldehyde	98-01-1	8.86E-02	9.19E-02	8.52E-02	1.05E-05	1.07E-05
2-heptanone	110-43-0	6.72E-02	7.19E-02	5.91E-02	7.54E-06	7.59E-06
2-methyl-1-butene	563-46-2	8.39E-02	9.51E-02	8.32E-02	9.45E-06	9.00E-06
2-methylfuran	534-22-5	9.10E-02	9.84E-02		1.05E-05	
2-methylthiophene	554-14-3	8.42E-02	8.74E-02		9.48E-06	
2-nitrotoluene (ONT)	88-72-2	7.11E-02	7.16E-02	5.70E-02	8.02E-06	8.50E-06
2-pentanone	107-87-9	7.98E-02	8.67E-02	7.80E-02	9.10E-06	9.07E-06
2-propanol	67-63-0	9.99E-02	1.07E-01	1.01E-01	1.13E-05	1.11E-05
2-thiophenecarboxaldehyde	98-03-3	8.25E-02	8.28E-02		9.48E-06	
3-(phenylhydrazone)-1H-indole-2,3-dione	17310-26-8					
3-furaldehyde	498-60-2	8.86E-02	9.27E-02		1.05E-05	
3-methyl-1-butene	563-45-1	8.39E-02	9.58E-02	8.36E-02	9.45E-06	8.91E-06
3-methylfuran	930-27-8	9.10E-02	9.84E-02		1.05E-05	
3-methylthiophene	616-44-4	8.42E-02	8.74E-02		9.48E-06	
3-nitrotoluene	99-08-1	7.11E-02	7.13E-02	5.72E-02	8.02E-06	8.51E-06
4-1,2,4-oxadizaolin-3-one-2,5-diphenyl-delta	Unknown					
4-amino-2,6-dinitrotoluene (4ADNT)	19406-51-0	6.44E-02	5.95E-02		6.90E-06	
4-ethyltoluene	622-96-8	6.62E-02	7.13E-02		7.55E-06	
4-methyl-2-pentanone	108-10-1	7.27E-02	7.89E-02	6.83E-02	8.22E-06	8.26E-06
4-nitrotoluene	99-99-0	7.11E-02	7.11E-02	7.25E-02	8.02E-06	

(Sheet 2 of 5)

Table 8 (Continued)

Chemical	CAS Number	Diffusion in Air			Diffusion in Water	
		Da_{FSG}	Da_{WL}	Da_{Water9}	Dw_{HL}	Dw_{Water9}
4-phenoxy-2(1H)-quinolinone	66662-28-0	5.27E-02	5.13E-02		5.93E-06	
acenaphthene	83-32-9	6.38E-02	6.46E-02	6.28E-02	7.27E-06	
acenaphthylene	208-96-8	6.46E-02	6.59E-02	4.29E-02	7.46E-06	
acetaldehyde	75-07-0	1.25E-01	1.38E-01	1.22E-01	1.48E-05	1.32E-05
acetic acid	64-19-7	1.13E-01	1.12E-01	1.17E-01	1.26E-05	1.34E-05
acetone	67-64-1	1.03E-01	1.13E-01	1.04E-01	1.20E-05	1.13E-05
acetonitrile	75-05-8	1.28E-01	1.31E-01	1.27E-01	1.41E-05	1.37E-05
acetophenone	98-86-2	7.02E-02	7.44E-02	6.21E-02	8.23E-06	8.45E-06
acetylene	74-86-2	1.53E-01	1.88E-01	8.49E-02	1.80E-05	1.03E-05
acrolein	107-02-8	1.06E-01	1.18E-01	1.09E-01	1.28E-05	1.20E-05
acrylonitrile	107-13-1	1.08E-01	1.15E-01	1.14E-01	1.23E-05	1.23E-05
aluminum^{3+}	7429-90-5					
anthracene	120-12-7	5.80E-02	5.84E-02	3.89E-02	6.63E-06	
antimony	7440-36-0			1.35E-01		
arsenic	7440-38-2			1.89E-01		
barium^{2+}	7440-39-3					
benzaldehyde	100-52-7	7.64E-02	8.17E-02	7.10E-02	9.10E-06	9.20E-06
benzanthrone (b)	82-05-3	5.29E-02	5.26E-02		6.06E-06	
benzene	71-43-2	8.69E-02	9.66E-02	8.52E-02	1.03E-05	9.93E-06
benzo(a)anthracene	56-55-3	5.13E-02	5.07E-02		5.85E-06	
benzo(a)pyrene	50-32-8	4.98E-02	5.14E-02		5.65E-06	
benzo(b)fluoranthene	205-99-2	4.98E-02	5.02E-02		5.61E-06	
benzo(e)pyrene	192-97-2	4.98E-02	5.14E-02		5.65E-06	
benzo(g,h,i)perylene	191-24-2	4.85E-02	4.62E-02		5.48E-06	
benzo(k)fluoranthene	207-08-9	4.98E-02	4.82E-02		5.61E-06	
benzofuran	271-89-6	7.13E-02	8.64E-02	6.82E-02	8.96E-06	9.13E-06
benzonitrile	100-47-0	7.72E-02	8.02E-02	7.17E-02	8.91E-06	9.14E-06
beryllium^{2+}	7440-41-7			4.70E-01		
bis(2-ethylhexyl)phthalate	117-81-7	3.62E-02	3.80E-02		3.78E-06	4.12E-06
butanal	123-72-8	8.92E-02	9.78E-02	8.92E-02	1.03E-05	1.00E-05
cadmium^{2+}	7440-43-9			1.59E-01		
calcium^{2+}	7440-70-2			1.72E-01		
carbon dioxide (CO2)	124-38-9	1.51E-01	1.80E-01		2.06E-05	
carbon disulfide	75-15-0	1.10E-01	3.92E-02	1.04E-01	3.05E-06	1.28E-05
carbon monoxide (CO)	630-08-0	1.81E-01	2.46E-01	1.80E-01	2.44E-05	2.15E-05
carbon tetrachloride	56-23-5	7.95E-02	8.47E-02	5.57E-02	9.34E-06	9.62E-06
carbonyl sulfide	463-58-1	1.26E-01	1.42E-01	1.11E-01	1.55E-05	1.29E-05
chlorobenzene	108-90-7	7.18E-02	7.94E-02	7.03E-02	8.53E-06	9.32E-06
chloroethene (vinyl chloride)	75-01-4	1.07E-01		1.04E-01	1.29E-05	1.18E-05
chloroform	67-66-3	8.85E-02	9.47E-02	7.51E-02	1.05E-05	1.07E-05
chloromethane	74-87-3	1.26E-01	1.40E-01	1.24E-01	1.50E-05	1.36E-05
chromium^{3+}	7440-47-3					
chrysene	218-01-9	5.13E-02	5.05E-02	1.39E-02	5.85E-06	
cis-2-butene	590-18-1	9.53E-02	1.09E-01		1.08E-05	
Cl2 (a)	7782-50-5	1.23E-01	1.35E-01	1.14E-01	1.53E-05	1.42E-05
cobalt^{2+}	7440-48-4					
copper^{2+}	7440-50-8					
dibenz(a,h)anthracene	53-70-3	4.65E-02	4.49E-02		5.24E-06	
dibenzo(b,def)chrysene-7,14 dione (c.i. vat yellow 4)	128-66-5	4.47E-02	4.29E-02		5.02E-06	
dibutyl phthalate	84-74-2	4.51E-02	4.57E-02		4.95E-06	5.24E-06
dichloroacetonitrile	3018-12-0	8.80E-02	9.06E-02	7.89E-02	1.02E-05	1.07E-05

(Sheet 3 of 5)

Table 8 (Continiued)

Chemical	CAS Number	Diffusion in Air			Diffusion in Water	
		Da_{FSG}	Da_{WL}	Da_{Water9}	Dw_{HL}	Dw_{Water9}
dichlorodiflouromethane	75-71-8		1.05E-01	5.61E-02	1.13E-05	8.85E-06
dimethyltrisulfide	3658-80-8	8.04E-02	7.77E-02		8.66E-06	
diphenylamine	122-39-4	5.89E-02	5.97E-02		6.67E-06	
ethane	74-84-0	1.37E-01	1.62E-01	1.15E-01	1.48E-05	1.11E-05
ethanol	64-17-5	1.20E-01	1.26E-01	1.21E-01	1.37E-05	1.30E-05
ethyl benzene	100-41-4	7.15E-02	7.77E-02	6.69E-02	8.23E-06	8.34E-06
ethyl chloride	75-00-3	1.04E-01	1.15E-01	9.23E-02	1.21E-05	1.09E-05
ethylene	74-85-1	1.45E-01	1.76E-01	6.50E-02	1.62E-05	8.30E-06
fluoranthene	206-44-0	5.58E-02	5.53E-02	2.34E-02	6.36E-06	
fluorene	86-73-7	6.07E-02	6.17E-02	3.86E-02	6.93E-06	
formaldehyde	50-00-0	1.68E-01	1.87E-01		2.06E-05	
furan	110-00-9	1.05E-01	1.14E-01	9.92E-02	1.24E-05	1.14E-05
HCl	7647-01-0	1.71E-01	1.91E-01	1.61E-01	2.11E-05	1.83E-05
heptanal	111-71-7	6.72E-02	7.19E-02	5.92E-02	7.54E-06	7.60E-06
hexachlorobenzene	118-74-1	5.57E-02	5.51E-02		6.29E-06	
hexachlorobutadiene	87-68-3	5.77E-02	5.95E-02		6.55E-06	7.03E-06
hexachlorocyclopentadiene	77-47-4	5.81E-02	5.88E-02		6.55E-06	7.22E-06
hexachloroethane	67-72-1	6.34E-02	6.57E-02	1.25E-02	7.17E-06	
hexanal	66-25-1	7.27E-02	7.83E-02	6.94E-02	8.22E-06	8.43E-06
hexane	110-54-3	7.44E-02	8.23E-02	7.28E-02	8.22E-06	8.12E-06
HMX	2691-41-0	7.14E-02	6.77E-02		8.87E-06	
hydrogen cyanide	74-90-8	1.77E-01	1.77E-01	1.68E-01	1.89E-05	1.68E-05
i-butane (isobutane)	75-28-5	9.29E-02	1.06E-01	8.91E-02	1.03E-05	9.18E-06
i-butene (isobutene/e-butylene)	115-11-7	9.53E-02	1.10E-01	9.60E-02	1.08E-05	9.86E-06
indeno(1,2,3-cd)pyrene	193-39-5	4.85E-02	4.61E-02		5.44E-06	
isothiocyanatomethane	556-61-6	1.03E-01	1.02E-01	1.09E-01	1.13E-05	
$lead^{2+}$	7439-92-1			5.77E-02		
xylene (mixed isomers)	1330-20-7	7.15E-02	7.76E-02		8.23E-06	4.30E-06
m-xylene (meta-xylene)	108-38-3	7.15E-02	7.68E-02	6.52E-02	8.23E-06	8.21E-06
p-xylene (para-xylene)	106-42-3	7.15E-02	7.76E-02	6.67E-02	8.23E-06	8.31E-06
$magnesium^{2+}$	7439-95-4			2.44E-01		
$manganese^{2+}$	7439-96-5					
m-dichlorobenzene	541-73-1	7.07E-02	7.47E-02	5.44E-02	8.32E-06	8.70E-06
mercury	7439-97-6			7.09E-02		3.01E-05
methacrolein	78-85-3	1.01E-01	9.68E-02	9.58E-02	1.14E-05	1.07E-05
methane	74-82-8	2.05E-01	2.50E-01		2.06E-05	
methylene chloride	75-09-2	1.02E-01	1.10E-01	9.74E-02	1.23E-05	1.23E-05
methylnitrite	624-91-9	1.25E-01	1.28E-01		1.38E-05	
methyl-t-butylether (MTBE)	1634-04-4	7.83E-02	8.56E-02	7.36E-02	8.63E-06	8.48E-06
methyl-vinyl ketone	78-94-4	9.13E-02	1.01E-01	9.41E-02	1.08E-05	1.07E-05
naphthalene	91-20-3	6.82E-02	7.19E-02	6.24E-02	7.99E-06	
n-butane	106-97-8	9.29E-02	1.06E-01	9.06E-02	1.03E-05	9.39E-06
n-decane	124-18-5	5.66E-02	6.02E-02	4.41E-02	6.16E-06	6.31E-06
NH3 (ammonia)	7664-41-7	2.55E-01	2.42E-01		2.48E-05	
$nickel^{2+}$	7440-02-0					
nitric acid	7697-37-2	1.48E-01	1.33E-01		1.63E-05	
nitrobenzene	98-95-3	7.21E-02	7.26E-02	6.63E-02	8.83E-06	9.29E-06
nitrogen oxide (NOx)	10102-44-0	1.77E-01	7.14E-02	1.54E-01	5.74E-06	1.87E-05
nitroglycerine	55-63-0	6.86E-02	6.21E-02	1.64E-02	7.01E-06	7.74E-06
nitromethane	75-52-5	1.25E-01	1.20E-01	1.19E-01	1.38E-05	1.39E-05
nonanal	124-19-6	5.91E-02	6.24E-02		6.54E-06	
OCDD (1,2,3,4,6,7,8,9-OCDD)	3268-87-9	4.46E-02	4.17E-02		4.85E-06	

(Sheet 4 of 5)

Table 8 (Concluded)

Chemical	CAS Number	Diffusion in Air			Diffusion in Water	
		Da_{FSG}	Da_{WL}	Da_{Water9}	Dw_{HL}	DwW_{ater9}
octanal	124-13-0	6.28E-02	6.70E-02	5.33E-02	6.99E-06	7.21E-06
o-dichlorobenzene	95-50-1	7.07E-02	7.44E-02	5.48E-02	8.32E-06	8.77E-06
o-methoxy-phenyl-azo-b-naphthol (oil red g)	1229-55-6	4.81E-02	4.61E-02		5.22E-06	
o-xylene (ortho-xylene)	95-47-6	7.15E-02	7.73E-02	6.74E-02	8.23E-06	8.41E-06
particulate cyanide	57-12-5					
p-dichlorobenzene (para-dichlorobenzene)	106-46-7	7.07E-02	7.56E-02	5.37E-02	8.32E-06	
pentaerythritoltetranitrate (PETN)	78-11-5	5.67E-02	4.99E-02		5.65E-06	
perchloroethylene	127-18-4	7.39E-02	7.82E-02	4.92E-02	8.69E-06	9.30E-06
phenanthrene	85-01-8	5.80E-02	5.88E-02	3.09E-02	6.69E-06	
phenol	108-95-2	8.28E-02	8.72E-02		9.85E-06	
phenylacetylene (ethynyl benzene)	536-74-3	7.37E-02	8.13E-02		8.78E-06	
phosphorus	7723-14-0					
propanal	123-38-6	1.03E-01	1.13E-01	1.10E-01	1.20E-05	1.22E-05
propane	74-98-6	1.09E-01	1.26E-01	7.57E-02	1.20E-05	8.69E-06
propylene	115-07-1	1.13E-01	1.33E-01	1.08E-01	1.28E-05	1.06E-05
propyne	74-99-7	1.17E-01	1.38E-01	8.45E-02	1.37E-05	1.01E-05
pyrene	129-00-0	5.58E-02	5.53E-02	2.66E-02	6.42E-06	
RDX	121-82-4	7.32E-02	6.01E-02	1.97E-02	7.07E-06	
selenium^{6+}	7782-49-2					
silver^{1+}	7440-22-4			1.66E-01		
styrene (vinyl benzene)	100-42-5	7.26E-02	7.92E-02	6.95E-02	8.49E-06	8.66E-06
sulfur dioxide (SO2)	7446-09-5	1.40E-01	1.42E-01		1.67E-05	
sulfuric acid	7664-93-9	1.14E-01	9.86E-02		1.28E-05	
tetryl (2,4,6-trinitrophenylmethylnitramine)	479-45-8	5.82E-02	5.51E-02		5.84E-06	
thallium^{4+}	7440-28-0					
thiophene	110-02-1	9.52E-02	1.03E-01	8.95E-02	1.15E-05	1.08E-05
toluene	108-88-3	7.81E-02	8.57E-02	7.59E-02	9.10E-06	9.06E-06
trans-2-butenal	123-73-9	9.13E-02	9.99E-02	9.43E-02	1.08E-05	1.07E-05
trans-2-butene	624-64-6	9.53E-02	1.10E-01	9.67E-02	1.08E-05	9.96E-06
trans-2-pentene	646-04-8	8.39E-02	9.48E-02	8.49E-02	9.45E-06	9.09E-06
trans-3-penten-2-one	625-33-2	8.13E-02	8.83E-02		9.45E-06	
trichloroethylene (TCE)	79-01-6	8.09E-02	8.72E-02	6.69E-02	9.65E-06	1.00E-05
trichloroflouromethane	75-69-4		9.36E-02	6.29E-02	1.02E-05	9.81E-06
vinylidenechloride	75-35-4	9.09E-02	1.09E-01	8.41E-02	1.23E-05	1.08E-05
zinc^{2+}	7440-66-6			2.19E-01		

(Sheet 5 of 5)

Data gaps

The methods listed above were used to calculate values for the diffusion coefficient where literature values were not available. However, there were a number of chemicals for which diffusion coefficients could not be calculated--including most of the trace metals. Most of the available methods for calculating the diffusion coefficient, whether in air or water, are oriented toward organic chemicals. The FSG, Wilke-Lee, and Hayduk and Laudie methods all require that a molar volume be calculated using the LeBas method. This can only be done for chemicals that are formed from elements that have known molar volume increments. If a chemical contains some atoms that do not have known molar volume increments, the total molar volume can be estimated as 85 to 90 percent

of the calculated LeBas molar volume. These methods, however, do not work for complex organic compounds or simple inorganic chemicals and trace metals for which molar volume increments have not yet been determined.

The simpler methods given in the WATER9 documentation (USEPA 1994) are also inclined toward organic compounds but require only molecular weight and a vapor or liquid density for the calculation. However, since there are no known liquid densities for many chemicals, such as trace metals that are only slightly soluble in water, these methods still do not provide a way to calculate the diffusion coefficient for all classes. Additional research would be required to determine if there is a method available that would allow for calculation of the diffusion coefficient for water-soluble forms of the trace metals.

Although no values could be calculated for many of the trace metals, diffusion coefficients in water for specific valence states for all of these were found in the literature. The values found for aluminum (Al^{3+}), barium (Ba^{2+}), magnesium (Mg^{2+}), manganese (Mn^{2+}), silver (Ag^{1+}), beryllium (Be^{2+}), nickel (Ni^{2+}), and thallium (Th^{4+}) should be applicable to most water bodies, but they were originally derived for interactions in seawater and deep-sea sediments (Li and Gregory 1974). However, none of the formulas that were examined for the calculation of diffusion coefficients in water indicate if the values are applicable for fresh water, seawater, or both.

4 Human Exposure Parameters

Introduction

In evaluating the risks presented by dermal and ingestion exposure to chemicals, it is essential to know the aqueous skin permeability constant (cm/hr), the gastrointestinal absorption fraction (GI absorption fraction, or GI ABS), and the fraction of contaminant absorbed through the skin as a result of soil dermal contact (dermal absorption fraction for soil). These three parameters are listed in Table 2 under human exposure parameters and are evaluated in this chapter.

Although data measurements are preferred, such measurements are expensive and often limited. This chapter describes alternative estimating methods using mathematical models and physicochemical properties to calculate human exposure parameters.

Methods

A search of methods was carried out using Internet Web sites and literature, such as *Environmental Science and Technology, Chemosphere, Environmental Toxicology and Chemistry, Environmental Pollution, SAR and QSAR in Environmental Research*, and USEPA reports. Available databases, such as RAIS (http://risk.lsd.ornl.gov/cgi-bin/tox/TOX_select?select=csfand), were also searched for information.

Aqueous Skin Permeability, K_p

The aqueous skin permeability constant (cm/hr) measures rate of absorption of a pollutant through skin for exposure pathways involving dermal contact with aqueous solutions. Showering and swimming are typical exposure pathways requiring the skin permeability constant to estimate dermal absorption. The USEPA summarizes values for permeability constants for selected chemicals (USEPA 1992a). For the chemical listed in the Range Database, USEPA values are used if available. For those chemicals in the Range Database that do not have values for K_p, a value can be estimated.

Models for skin permeability

Regression equations for the prediction of K_p values from partition coefficients and/or molecular weight values have long been available, but generally these regressions were developed for specific sets or classes of compounds. Guy and Hadgraft (1989) explored the validity of using a regression equation derived empirically for one class of compounds under a set of defined experimental conditions to predict the K_p values for a compound in a structurally dissimilar class. They found that when the K_p values for phenols are compared to the predictions obtained by the equation developed by Lien and Tong (1973) for alkanols, there is a tendency to overestimate the absorption values for the phenols, with the most marked deviation in predictions of K_p for phenols with log K_{ow} < 2.0.

Flynn (1990) compiled a database composed of about 90 hydrocarbon compounds evaluated for absorption from water through human skin in vitro. The Flynn database has been subjected to independent analyses by several investigators including Potts and Guy (1992) to fit these data to equations that account for both molecular size and polarity, the latter as determined by K_{ow}. Flynn (1990) provides different equations for calculating K_p for different K_{ow} and MW ranges (Table 9). However, K_p estimations may be inaccurate for chemicals with K_{ow} and MW values outside the range of those in the Flynn database or for highly lipophilic and halogenated chemicals as well as for compounds which are partially or completely ionized. The K_p of two classes of chemicals with very low K_{ow} and very high K_{ow} were found not to correlate well with log K_{ow} (Leahy 1990).

Table 9
Algorithms for Calculating Permeability Coefficient, K_p, from Octanol/Water Coefficient

Range of K_{ow}	Low Molecular Weight Compounds (<150)	High Molecular Weight Compounds (>150)
log K_{ow} < 0.5	log K_p = -3	log K_p = -5
0.5<log K_{ow} < 3.0	log K_p = -3+log K_{ow}	log K_p = -5.5+log K_{ow}
log K_{ow} > 3.0	log K_p = -0.5	log K_p = -1.5

Source: Flynn (1990).

Anatomically based, physical models provide an alternative to the empirical approaches for obtaining K_p values (Kasting et al. 1987), and such models may offer a better alternative for predicting K_p from known physicochemical properties. The anatomically based, physical models are important because they place skin permeability in terms of parallel pathways and series barriers. Although these types of models potentially offer innovative approaches for estimating skin permeability, they are presently still considered a developing method, so are not used in this study but should be considered at some future time. For now, empirical correlation models are recommended.

Equations for estimating K_p for organics

Potts and Guy (1992) proposed an empirical correlation for estimating K_p that is a function of K_{ow} and MW and is based on the experimental database of Flynn (1990),

$$\log K_p = -2.72 + 0.71 \times \log K_{ow} - 0.0061 \times \mathrm{MW} \qquad (15)$$

USEPA (1992a) recommends that Equation 15 be used within the "effective prediction domain" (EPD) that has been determined via a statistical analysis (Figure 1). Estimated values of K_p for chemicals that are outside of the EPD may be suspect. Equation 15 was used for the Range Database to estimate K_p and is recommended until more comprehensive equations can be developed. Additionally, Equation 15 is used in the ARAMS/FRAMES constituent database editor to estimate K_p.

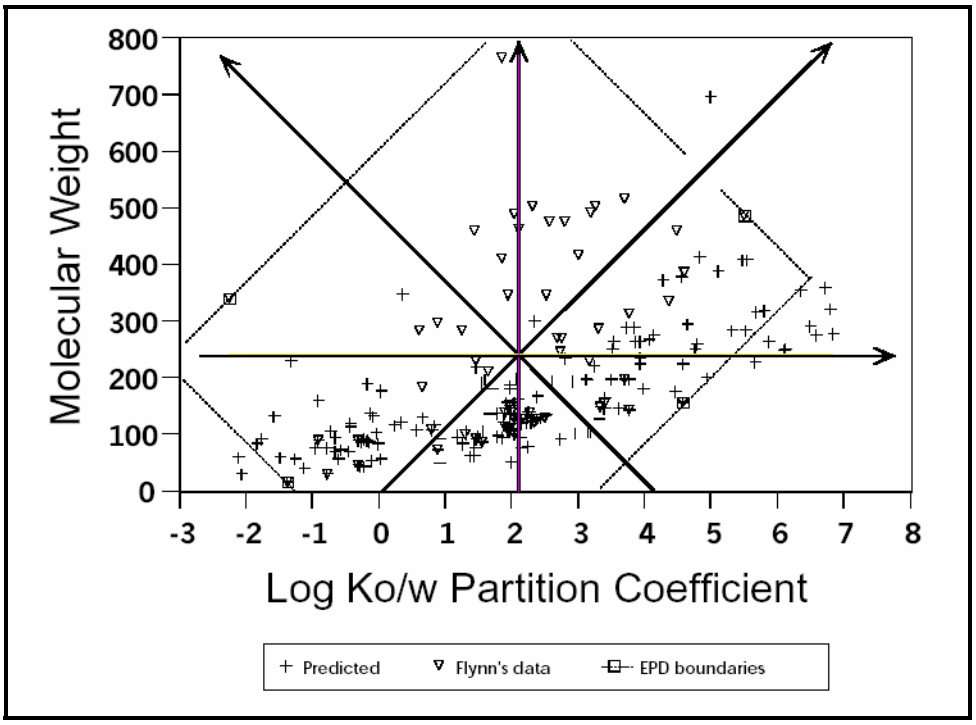


Figure 1. EPD boundaries for *Kp* estimation (USEPA 2004b). (*Ko/w* is same as the K_{ow} used in this report)

McKone and Howd (1992) developed an alternative equation to Equation 15:

$$K_p = \mathrm{MW}^{-0.6}\left[0.33 + \frac{0.0025}{2.4\times10^{-6} + 3\times10^{-5}\,K_{ow}^{0.8}}\right]^{-1} \qquad (16)$$

Equations 15 and 16 were used to compute K_p values for selected chemicals and results were compared with experimentally determined values (Table 10). The calculated error (AME) shows that, for these chemicals, Equation 16 has a

lower AME, which means it calculates K_p closer to measured data than Equation 15. The chemicals in Table 10 all have log K_{ow} less than 6. The difference between these computed and measured values could be due to experimental or analytical error. Vecchia (1997) found that replicated experimental measurements often vary by one to two orders of magnitude. Although Equation 16 is slightly more accurate than Equation 15, Equation 15 was used to generate values for the Range Database since USEPA recommends this equation.

Table 10
Comparison of K_p (cm/hr) Estimates from Equations 15 and 16

Chemical	CAS Number	Measured K_p	Calculated K_p from Eq. 15	Calculated K_p from Eq. 16
1-butanol	71-36-3	0.0025	0.0019	0.0036
2-butanone	78-93-3	0.0050	0.0011	0.0016
benzene	71-43-2	0.1100	0.0210	0.0365
carbon disulfide	75-15-0	0.5000	0.0240	0.0307
chloroform	67-66-3	0.1300	0.0089	0.0224
ethanol	64-17-5	0.0008	0.0006	0.0008
perchloroethylene	127-18-4	0.3700	0.0480	0.0455
phenol	108-95-2	0.0082	0.0055	0.0110
styrene (vinyl benzene)	100-42-5	0.6700	0.0550	0.0888
tetrachloroethene	127-18-4	0.3700	0.0480	0.0455
toluene	108-88-3	1.0000	0.0450	0.0757
trichloroethylene (TCE)	79-01-6	0.2300	0.0160	0.0414
AME			73.6315	69.1547

Estimating K_p for inorganics

Table 11 summarizes experimentally determined permeability coefficients for several inorganic compounds (data of Hostynek et al. (1998) reported by

Table 11
Permeability Coefficients for Inorganics

Compound	K_p, cm/hr
cadmium	1×10^{-3}
chromium (+6)	2×10^{-3}
chromium (+3)	1×10^{-3}
cobalt	4×10^{-4}
lead	1×10^{-4}
mercury (+2)	1×10^{-3}
methyl mercury	1×10^{-3}
mercury vapor	0.24
nickel	2×10^{-4}
potassium	2×10^{-3}
silver	6×10^{-4}
zinc	6×10^{-4}
all other inorganics	1×10^{-3}

USEPA 1992a). To be most protective of human health, the values listed in Table 11 represent the highest reported permeability coefficient. More detailed information is presented in USEPA (1992a). The default value for other inorganic chemicals is 10^{-3} cm/hr.

GI Absorption Fraction

GI absorption fraction (GI ABS, dimensionless) is the fraction of contaminant that is absorbed in the gastrointestinal tract. This parameter is used to derive the dermal toxicity from oral toxicity values for chemicals. The GI ABS is used to adjust oral toxicity values for the assessment of dermal contact. As the GI value decreases, the dermal pathway to overall risk relative to the ingestion pathway increases. Therefore, the GI can greatly influence the comparative importance of the dermal pathway in a risk assessment.

USEPA (2005) recommended GI absorption values for selected compounds (Table 12). USEPA Region 4 (USEPA 1995d) recommends default GI ABS values of 0.8 for volatile organics, 0.5 for semivolatile organics, and 0.2 for inorganic chemicals when measured values are not available.

Table 12
Summary of Recommended Gastrointestinal Absorption Fractions for Specific Compounds

Compound	Reference[1]	Species	Dosing Regimen	GI ABS (fraction)
chlordane	Ewing, 1985 Ohno, 1986	Rat	Assume aqueous gavage	0.80
2,4 dichlorophenoxyacetic acid (2,4-D)	Knopp, 1992 Pelletier, 1989	Rat	Assume aqueous gavage	>0.90
DDT	Keller, 1980	Rat	Vegetable oil	0.70-0.90
pentachlorophenol	Korte, 1978	Rat	Diet	0.76
	Meerman, 1983	Rat	Water	1.00
polychlorinated biphenyls (PCBs)	Albro, 1972	Rat	Squalene	0.96
	Muhlebach, 1981	Rat	Emulsion	0.80
	Tanabe, 1981	Rat	Corn oil	0.81
polycyclic aromatic hydrocarbons (PAHs)	Chang, 1943	Rat	Starch solution	0.58
	Hecht, 1979	Rat	Diet	0.89
TCDD	Fries, 1975	Rat	Diet	0.50-0.60
	Piper, 1973	Rat	Diet	0.70
	Rose, 1976	Rat	Corn oil	0.70-0.83
other dioxins/dibenzofurans	ATSDR, 1994a	Multiple studies		>0.50
all other organic compounds	Multiple references			Generally > 0.50
Inorganics				
antimony	Waitz, 1965	Rat	Water	0.15
arsenic (arsenite)	Bettley, 1975	Human	Assume aqueous	0.95
barium	Cuddihy and Griffith 1972 Taylor, 1962	Dog	Water	0.07
beryllium	Reeves, 1965	Rat	Water	0.007

(Continued)

[1] Literature references are listed by first author (Source: USEPA 2004b).

Table 12 (Concluded)

Compound	Reference	Species	Dosing Regimen	GI ABS (fraction)
Inorganics (Concluded)				
cadmium	IRIS, 2000	Human	Diet	0.025
		Human	Water	0.05
chromium (III)	Donaldson and Barreras, 1996 Keim, 1987	Rat	Diet/water	0.013
chromium (VI)	Donaldson and Barreras, 1996 MacKenzie, 1959 Sayato, 1980	Rat	Water	0.025
cyanate	Farooqui and Ahmed 1982	Rat	Assume aqueous	>0.47
manganese	Davidsson, 1989 IRIS, 2000 Ruoff, 1995	Human	Diet/water	0.04
mercuric chloride (other soluble salts)	IRIS, 2000	Rat	Water	0.07
insoluble or metallic mercury	ASTDR, 1994b	Human	Acute inhalation of Hg vapor	0.74-0.80
methyl mercury	Aberg, 1969	Human	Aqueous	0.95
nickel	Elakhovskaya, 1972	Human	Diet/water	0.04
selenium	Young, 1982	Human	Diet	0.30-0.80
silver	Furchner, 1968	Dog	Aqueous	0.04
thallium	Lie, 1960	Rat	Aqueous	1.00
vanadium	Conklin, 1982	Rat	Gavage	0.026
zinc	ASTDR, 1994c	Human	Diet	Highly variable

Dermal Absorption Fraction from Soil

Dermal absorption fraction is the relative amount of a substance on the skin that penetrates through the epidermis into the body resulting from soil contact. Dermal contact with contaminated soil represents a potentially significant route of exposure to toxic compounds. A number of methodologies have been developed to estimate the exposure of an individual to toxic compounds in a soil matrix. One approach is to include an absorption factor to permit the calculation of absorbed dose (e.g., USEPA 1984; USEPA 1989). For most chemicals, the parameters in these approaches have not been well characterized. Major uncertainties exist in the extent to which a chemical is percutaneously absorbed and in the extent to which a chemical will partition from soil to skin. In addition, the absorption of a chemical in a soil matrix may depend on characteristics of the soil, such as particle size and organic carbon content, which affect partitioning of the chemical between soil and skin. For the dermal-soil pathway, the limited availability of dermal absorption values is expected to result in a limited number of contaminants being considered in a quantitative risk assessment.

Absorption of chemicals through the skin is thought to occur primarily via diffusion. Under ideal conditions (i.e., steady-state, homogeneous media, etc.) diffusion can be modeled with Fick's first law. Based on Fick's first law, the dermal absorption fraction (ABS) may be calculated (USEPA 2004b) from

$$ABS = \frac{\rho_{soil} t_{event} \dfrac{D_s}{l_s}}{AF} K_{s/soil} \qquad (17)$$

where

ρ_{soil} = Density of soil (mg/cm^3)
t_{event} = Exposure time per event (hr/event)
D_s = Diffusivity of the chemical in skin (cm^2/hr)
l_s = Skin thickness (μm) x (10^{-4} cm/μm)
AF = Soil to skin adherence factor (mg/cm^2-event)
$K_{s/soil}$ = Skin/soil partition coefficient (unitless)

Processes occurring in the soil, such as desorption from and diffusion through the soil and volatilization, create a far more complex situation than described by Equation 17. Additionally, Equation 17 requires several parameters that must be measured, estimated, or computed, making the use of this equation problematic. Therefore, although Equation 17 is theoretically interesting, it is of little practical use for estimating dermal ABS.

Reported values of dermal ABS for selected chemicals are shown in Table 13 for use in the Range Database. USEPA (1992a) recommends using a value of 0.001 for inorganics and 0.01 for organics as default values when specific data are not available otherwise.

Table 13
Reported Dermal Absorption Fraction from Soil

Compound	Dermal Absorption Fraction	Reference
arsenic	0.03	Wester et al. (1993a)
cadmium	0.001	Wester et al. (1992a) USEPA (1992a)
chlordane	0.04	Wester et al. (1992b)
2,4-dichlorophenoxyacetic acid	0.05	Wester et al. (1996)
DDT	0.03	Wester et al. (1990)
TCDD and other dioxins -if soil organic content is >10%	0.03 0.001	USEPA (1992a)
lindane	0.04	Duff and Kissel (1996)
benzo(a)pyrene and other PAHs	0.13	Wester et al. (1990)
aroclors 1254/1242 and other PCBs	0.14	Wester et al. (1993b)
pentachlorophenol	0.25	Wester et al. (1993c)
semivolatile organic compounds	0.1	—

(Continued)

Table 13 (Concluded)

Compound	Dermal Absorption Fraction	Reference
Explosives		
hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX)	0.015	Reifenrath et al. (2002)
thiodiglycol	0.0075	Reifenrath et al. (2002)
trinitrobenzene	0.019	Reifenrath et al. (2002)
2,4-dinitrotoluene (2,4-DNT)	0.102	Reifenrath et al. (2002)
2,6-dinitrotoluene (2,6-DNT)	0.099	Reifenrath et al. (2002)
2-amino-4,6-dinitrotoluene (2a, 4,6-DNT)	0.006	Reifenrath et al. (2002)
4-amino-2,6-dinitrotoluene (4a, 2,6-DNT)	0.009	Reifenrath et al. (2002)
2,4-diamino-6-nitrotoluene (2,4-DA-6-NT)	0.011	Reifenrath et al. (2002)
2,6-diamino-4-nitrotoluene (2,6-DA, 4-NT)	0.005	Reifenrath et al. (2002)
trinitrotoluene (TNT)	0.032	Reifenrath et al. (2002)
octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX)	0.006	Reifenrath et al. (2002)
tetryl (n-methyl-n, 2,4,6-tetranitrobenzamine)	0.00065	Reifenrath et al. (2002)

Other Sources of Data

The ARAMS/FRAMES Database and the RAIS Database were searched for information on all three human exposure parameters. Table 14 shows available data from ARAMS/FRAMES and Table 15 provides data available from RAIS. RAIS has values for 60 percent (111) of the chemicals on the Range Database list, whereas ARAMS/FRAMES Database has only about 10 to 36 percent of the data for the Range chemicals. The RAIS Database includes default values, whereas the ARAMS/FRAMES Database does not. Values in Tables 14 and 15 will be added to the Range Database.

Table 14
Available Data for Human Exposure Parameters for Range Database Chemicals in the ARAMS/FRAMES Database

ID	Chemical	CAS Number	K_p, cm/hr	GI ABS (fraction)	Dermal ABS (fraction)
1	1,2-dichloroethene (cis)	156-59-2			
2	1,2-dichloroethene (trans)	156-60-5	1.00E-02		
3	(1,2-dichloroethyl) benzene	1074-11-9			
4	1,2,4-trimethylbenzene	95-63-6			
5	1,2-dichlorethane	107-06-2		9.00E-01	
6	1,2-dichloro-3-methylbenzene	32768-54-0			
7	1,2-dichloroethene (cis/trans mixture)	540-59-0			
8	1,3,5-trimethylbenzene (mesitylene)	108-67-8			
9	1,3,5-trinitrobenzene	99-35-4		5.00E-01	

(Sheet 1 of 6)

Table 14 (Continued)

ID	Chemical	CAS Number	K_p, cm/hr	GI ABS (fraction)	Dermal ABS (fraction)
10	1,3-butadiene	106-99-0			
11	1,3-dinitrobenzene	99-65-0		6.00E-01	
12	1,4-diamino-2,3-dihydroanthraquinone (DDA) violet-dye mix	81-63-0			
13	1,4-di-p-toluidinoanthraquinone (PTA) solvent green 3	128-80-3			
14	1-butanol	71-36-3	2.50E-03		
15	1-butene	106-98-9			
16	1-chloro-2-methylbenzene	95-49-8			
17	1-chloro-3-methylbenzene	108-41-8			
18	1-hexene	592-41-6			
19	1-pentene	109-67-1			
20	1-(methylamino)anthraquinone (disperse red 9)	82-38-2			
21	2-(2-quinolyl)-1,3-indandione (D & C yellow no. 11) or (solvent yellow 33)	8003-22-3			
22	2,3-butanedione	625-34-3			
23	2,3,7,8-tetrachlorodibenzo-p-dioxin	1746-01-6	1.40E+00		3.00E-02
24	2,4,6-trinitrotoluene (TNT)	118-96-7		2.00E-01	
25	2,4-dinitrotoluene (DNT; 2,4-DNT)	121-14-2		5.00E-01	
26	2,6-dinitrotoluene (2,6-DNT)	606-20-2			
27	2,5-dimethylfuran	625-86-5			
28	2-amino-4,6-dinitrotoluene	35572-78-2		5.00E-01	
29	2-amino-9,10-anthracenedione (a) (AAQ)	117-79-3			
30	2-butanone	78-93-3	5.00E-03		
31	2-furaldehyde	98-01-1			
32	2-heptanone	110-43-0			
33	2-methyl-1-butene	563-46-2			
34	2-methylfuran	534-22-5			
35	2-methylthiophene	554-14-3			
36	2-nitrotoluene (ONT)	88-72-2		5.00E-01	1.00E-01
37	2-pentanone	107-87-9			
38	2-propanol	67-63-0		8.00E-01	
39	2-thiophenecarboxaldehyde	98-03-3			
40	3-(phenylhydrazone)-1H-indole-2,3-dione				
41	3-furaldehyde	498-60-2			
42	3-methyl-1-butene	563-45-1			
43	3-methylfuran	930-27-8			
44	3-methylthiophene	616-44-4			
45	3-nitrotoluene	99-08-1			
46	4-1,2,4-oxadizaolin-3-one-2,5-diphenyl-delta				
47	4-amino-2,6-dinitrotoluene (4ADNT)	19406-51-0			
48	4-ethyltoluene	622-96-8			
49	4-methyl-2-pentanone	108-10-1	3.30E-03		
50	4-nitrotoluene	99-99-0			

(Sheet 2 of 6)

Table 14 (Continued)

ID	Chemical	CAS Number	K_p, cm/hr	GI ABS (fraction)	Dermal ABS (fraction)
51	4-phenoxy-2(1H)-quinolinone	66662-28-0			
52	acenaphthene	83-32-9		6.00E-01	1.30E-01
53	acenaphthylene	208-96-8		6.00E-01	
54	acetaldehyde	75-07-0			
55	acetic acid	64-19-7			
56	acetone	67-64-1		8.00E-01	
57	acetonitrile	75-05-8			
58	acetophenone	98-86-2			
59	acetylene	74-86-2			
60	acrolein	107-02-8	7.40E-04		
61	acrylonitrile	107-13-1		8.00E-01	
62	aluminum	7429-90-5	7.20E-06		
63	anthracene	120-12-7		6.00E-01	1.30E-01
64	antimony	7440-36-0		2.00E-01	
65	arsenic	7440-38-2		2.00E-01	4.50E-02
66	barium	7440-39-3		8.00E-02	
67	benzaldehyde	100-52-7		8.00E-01	
68	benzanthrone (b)	82-05-3			
69	benzene	71-43-2	1.10E-01	8.00E-01	
70	benzo(a)anthracene	56-55-3		8.00E-01	1.30E-01
71	benzo(a)pyrene	50-32-8		7.00E-01	1.30E-01
72	benzo(b)fluoranthene	205-99-2		7.00E-01	1.30E-01
73	benzo(e)pyrene	192-97-2		5.00E-01	1.30E-01
74	benzo(g,h,i)perylene	191-24-2			
75	benzo(k)fluoranthene	207-08-9		7.00E-01	1.30E-01
76	benzofuran	271-89-6			
77	benzonitrile	100-47-0			
78	beryllium	7440-41-7		6.00E-03	
79	bis(2-ethylhexyl)phthalate	117-81-7		2.00E-01	
80	butanal	123-72-8			
81	cadmium	7440-43-9	1.00E-03	5.00E-02	1.00E-03
82	calcium	7440-70-2		3.00E-01	
83	carbon dioxide (CO2)	124-38-9			
84	carbon disulfide	75-15-0	5.00E-01		
85	carbon monoxide (CO)	630-08-0			
86	carbon tetrachloride	56-23-5	2.20E-02		
87	carbonyl sulfide	463-58-1			
88	chlorobenzene	108-90-7	4.10E-02		
89	chloroethene (vinyl chloride)	75-01-4	7.30E-03		
90	chloroform	67-66-3	1.30E-01	8.00E-01	
91	chloromethane	74-87-3	4.20E-03	8.00E-01	

(Sheet 3 of 6)

Table 14 (Continued)

ID	Chemical	CAS Number	K_p, cm/hr	GI ABS (fraction)	Dermal ABS (fraction)
92	chromium	7440-47-3	2.00E-03	2.00E-02	
93	chrysene	218-01-9		8.00E-01	1.30E-01
94	cis-2-butene	590-18-1			
95	Cl2 (a)	7782-50-5			
96	cobalt	7440-48-4	4.00E-04	3.00E-01	
97	copper	7440-50-8		6.00E-01	
98	dibenz(a,h)anthracene	53-70-3		7.00E-01	1.30E-01
99	dibenzo(b,def)chrysene-7,14 dione (c.i. vat yellow 4)	128-66-5			
100	dibutyl phthalate	84-74-2		5.00E-01	
101	dichloroacetonitrile	3018-12-0			
102	dichlorodiflouromethane	75-71-8	1.20E-02		
103	dimethyltrisulfide	3658-80-8			
104	diphenylamine	122-39-4			
105	ethane	74-84-0			
106	ethanol	64-17-5	8.00E-04		
107	ethyl benzene	100-41-4	1.00E+00		
108	ethyl chloride	75-00-3	8.00E-03		
109	ethylene	74-85-1			
110	fluoranthene	206-44-0		6.00E-01	1.30E-01
111	fluorene	86-73-7		6.00E-01	1.30E-01
112	formaldehyde	50-00-0	2.20E-03		
113	furan	110-00-9			
114	HCl	7647-01-0		1.00E+00	
115	heptanal	111-71-7			
116	hexachlorobenzene	118-74-1	2.10E-01		
117	hexachlorobutadiene	87-68-3	1.20E-01		
118	hexachlorocyclopentadiene	77-47-4			
119	hexachloroethane	67-72-1	4.20E-02		
120	hexanal	66-25-1			
121	hexane	110-54-3		8.00E-01	
122	HMX	2691-41-0		5.00E-01	
123	hydrogen cyanide	74-90-8			
124	i-butane (isobutane)	75-28-5			
125	i-butene (isobutene/e-butylene)	115-11-7			
126	indeno(1,2,3-cd)pyrene	193-39-5		7.00E-01	1.30E-01
127	isothiocyanatomethane	556-61-6			
128	lead	7439-92-1	4.00E-06	3.00E-01	
129	xylene (mixed isomers)	1330-20-7		8.00E-01	
130	m-xylene (meta-xylene)	108-38-3		8.00E-01	
131	p-xylene (para-xylene)	106-42-3		8.00E-01	
132	magnesium	7439-95-4			

(Sheet 4 of 6)

Table 14 (Continued)

ID	Chemical	CAS Number	K_p, cm/hr	GI ABS (fraction)	Dermal ABS (fraction)
133	manganese	7439-96-5		1.00E-01	
134	m-dichlorobenzene	541-73-1	8.70E-02		
135	mercury	7439-97-6	1.00E-03	1.50E-01	
136	methacrolein	78-85-3			
137	methane	74-82-8			
138	methylene chloride	75-09-2		7.00E-01	
139	methylnitrite	624-91-9			
140	methyl-t-butylether (MTBE)	1634-04-4			
141	methyl-vinyl ketone	78-94-4			
142	naphthalene	91-20-3		8.00E-01	
143	n-butane	106-97-8			
144	n-decane	124-18-5			
145	NH3 (ammonia)	7664-41-7		5.00E-01	
146	nickel	7440-02-0	1.00E-04	3.00E-01	
147	nitric acid	7697-37-2			
148	nitrobenzene	98-95-3		5.00E-01	
149	nitrogen oxide (NOx)	10102-44-0			
150	nitroglycerine	55-63-0			
151	nitromethane	75-52-5			
152	nonanal	124-19-6		5.00E-01	
153	OCDD (1,2,3,4,6,7,8,9-OCDD)	3268-87-9		5.00E-01	
154	octanal	124-13-0			
155	o-dichlorobenzene	95-50-1	6.10E-02		
156	o-methoxy-phenyl-azo-b-naphthol (oil red g)	1229-55-6			
157	o-xylene (ortho-xylene)	95-47-6		8.00E-01	
158	particulate cyanide	57-12-5			
159	p-dichlorobenzene (para-dichlorobenzene)	106-46-7	6.20E-02		
160	pentaerythritoltetranitrate (PETN)	78-11-5			
161	perchloroethylene	127-18-4	3.70E-01	8.00E-01	
162	phenanthrene	85-01-8		6.00E-01	1.30E-01
163	phenol	108-95-2	8.20E-03		
164	phenylacetylene (ethynyl benzene)	536-74-3			
165	phosphorus	7723-14-0		8.00E-01	
166	propanal	123-38-6			
167	propane	74-98-6			
168	propylene	115-07-1			
169	propyne	74-99-7			
170	pyrene	129-00-0		8.00E-01	1.30E-01
171	RDX	121-82-4		5.00E-01	
172	selenium	7782-49-2		5.00E-02	
173	silver	7440-22-4	6.00E-04	2.00E-01	

(Sheet 5 of 6)

Table 14 (Concluded)

ID	Chemical	CAS Number	K_p, cm/hr	GI ABS (fraction)	Dermal ABS (fraction)
174	styrene (vinyl benzene)	100-42-5	6.70E-01		
175	sulfur dioxide (SO2)	7446-09-5			
176	sulfuric acid	7664-93-9			
177	tetryl (2,4,6-trinitrophenylmethylnitramine)	479-45-8		5.00E-01	1.00E-01
178	thallium	7440-28-0		1.00E+00	
179	thiophene	110-02-1			
180	toluene	108-88-3		8.00E-01	
181	trans-2-butenal	123-73-9			
182	trans-2-butene	624-64-6			
183	trans-2-pentene	646-04-8			
184	trans-3-penten-2-one	625-33-2			
185	trichloroethylene (TCE)	79-01-6	2.30E-01	9.00E-01	
186	trichloroflouromethane	75-69-4	1.70E-02		
187	vinylidenechloride	75-35-4	1.60E-02		
188	zinc	7440-66-6	6.00E-04	2.00E-01	
Statistical Summary					
Number of available data values			39	67	19
Number of not available data			149	121	169
Percent available data			21	36	10

(Sheet 6 of 6)

Table 15
Available Data for Human Exposure Parameters for Range Database Chemicals in the RAIS Database

ID	Chemical	CAS Number	K_p, cm/hr	GI ABS (fraction)	Dermal ABS (fraction)
1	1,2-dichloroethene (cis)	156-59-2	0.0149	1	0.01
2	1,2-dichloroethene (trans)	156-60-5	0.0149	1	0.01
3	(1,2-dichloroethyl) benzene	1074-11-9			
4	1,2,4-trimethylbenzene	95-63-6	0.133	0.8	0.01
5	1,2-dichlorethane	107-06-2	0.00534	1	0.01
6	1,2-dichloro-3-methylbenzene	32768-54-0			
7	1,2-dichloroethene (cis/trans mixture)	540-59-0	0.0149	0.8	0.01
8	1,3,5-trimethylbenzene (mesitylene)	108-67-8	0.0944	0.8	0.01
9	1,3,5-trinitrobenzene	99-35-4	0.000657	0.65	0.01
10	1,3-butadiene	106-99-0	0.0231	0.8	0.01
11	1,3-dinitrobenzene	99-65-0	0.00205	0.65	0.01
12	1,4-diamino-2,3-dihydroanthraquinone (DDA) violet-dye mix	81-63-0			
13	1,4-di-p-toluidinoanthraquinone (PTA) solvent green 3	128-80-3			
14	1-butanol	71-36-3	0.00284	0.5	0.01

(Sheet 1 of 5)

Table 15 (Continued)

ID	Chemical	CAS Number	K_p, cm/hr	GI ABS (fraction)	Dermal ABS (fraction)
15	1-butene	106-98-9			
16	1-chloro-2-methylbenzene	95-49-8	0.0863	0.8	0.01
17	1-chloro-3-methylbenzene	108-41-8			
18	1-hexene	592-41-6			
19	1-pentene	109-67-1			
20	1-(methylamino)anthraquinone (disperse red 9)	82-38-2			
21	2-(2-quinolyl)-1,3-indandione (D & C yellow no. 11) or (solvent yellow 33)	8003-22-3			
22	2,3-butanedione	625-34-3			
23	2,3,7,8-tetrachlorodibenzo-p-dioxin	1746-01-6	1.39	0.5	0.03
24	2,4,6-trinitrotoluene (TNT)	118-96-7	0.00107	0.6	0.01
25	2,4-dinitrotoluene (DNT; 2,4-DNT)	121-14-2	0.00376	0.85	0.01
26	2,6-dinitrotoluene (2,6-DNT)	606-20-2	0.00457	0.85	0.01
27	2,5-dimethylfuran	625-86-5			
28	2-amino-4,6-dinitrotoluene	35572-78-2	0.00241	0.5	0.01
29	2-amino-9,10-anthracenedione (a) (AAQ)	117-79-3			
30	2-butanone	78-93-3	0.00111	0.8	0.01
31	2-furaldehyde	98-01-1	0.000966	0.5	0.01
32	2-heptanone	110-43-0			
33	2-methyl-1-butene	563-46-2			
34	2-methylfuran	534-22-5			
35	2-methylthiophene	554-14-3			
36	2-nitrotoluene (ONT)	88-72-2	0.0119	0.8	0.01
37	2-pentanone	107-87-9			
38	2-propanol	67-63-0	0.000889	1	0.01
39	2-thiophenecarboxaldehyde	98-03-3			
40	3-(phenylhydrazone)-1H-indole-2,3-dione				
41	3-furaldehyde	498-60-2			
42	3-methyl-1-butene	563-45-1			
43	3-methylfuran	930-27-8			
44	3-methylthiophene	616-44-4			
45	3-nitrotoluene	99-08-1	0.0152	0.8	0.01
46	4-1,2,4-oxadizaolin-3-one-2,5-diphenyl-delta				
47	4-amino-2,6-dinitrotoluene (4ADNT)	19406-51-0			
48	4-ethyltoluene	622-96-8			
49	4-methyl-2-pentanone	108-10-1	0.00397	0.8	0.01
50	4-nitrotoluene	99-99-0	0.0134	0.8	0.01
51	4-phenoxy-2(1H)-quinolinone	66662-28-0			
52	acenaphthene	83-32-9	0.133	0.31	0.13
53	acenaphthylene	208-96-8	0.141	0.31	0.01
54	acetaldehyde	75-07-0	0.000589	0.8	0.01
55	acetic acid	64-19-7			
56	acetone	67-64-1	0.000569	0.83	0.01
57	acetonitrile	75-05-8	0.000614	0.8	0.01
58	acetophenone	98-86-2	0.00467	0.8	0.01
59	acetylene	74-86-2			
60	acrolein	107-02-8	0.000853	0.8	0.01
61	acrylonitrile	107-13-1	0.00136	0.8	0.01

(Sheet 2 of 5)

Table 15 (Continued)

ID	Chemical	CAS Number	K_p, cm/hr	GI ABS (fraction)	Dermal ABS (fraction)
62	aluminum	7429-90-5	0.00214	0.1	0.001
63	anthracene	120-12-7	0.225	0.76	0.13
64	antimony	7440-36-0	0.00109	0.02	0.001
65	arsenic	7440-38-2	0.00193	0.41	0.03
66	barium	7440-39-3	0.000403	0.07	0.001
67	benzaldehyde	100-52-7	0.00482	0.8	0.01
68	benzanthrone (b)	82-05-3			
69	benzene	71-43-2	0.0207	0.97	0.01
70	benzo(a)anthracene	56-55-3	0.948	0.31	0.13
71	benzo(a)pyrene	50-32-8	1.24	0.31	0.13
72	benzo(b)fluoranthene	205-99-2	0.699	0.31	0.13
73	benzo(e)pyrene	192-97-2			
74	benzo(g,h,i)perylene	191-24-2	2	0.31	0.13
75	benzo(k)fluoranthene	207-08-9	1.2	0.31	0.13
76	benzofuran	271-89-6			
77	benzonitrile	100-47-0			
78	beryllium	7440-41-7	0.00066	0.01	0.001
79	bis(2-ethylhexyl)phthalate	117-81-7	1.97	0.19	0.01
80	butanal	123-72-8			
81	cadmium	7440-43-9	0.00035	0.01	0.001
82	calcium	7440-70-2			
83	carbon dioxide (CO2)	124-38-9			
84	carbon disulfide	75-15-0	0.0156	0.63	0.25
85	carbon monoxide (CO)	630-08-0			
86	carbon tetrachloride	56-23-5	0.0224	0.65	0.01
87	carbonyl sulfide	463-58-1			
88	chlorobenzene	108-90-7	0.0407	0.31	0.01
89	chloroethene (vinyl chloride)	75-01-4	0.0113	1	0.01
90	chloroform	67-66-3	0.00892	0.2	0.01
91	chloromethane	74-87-3	0.00415	0.8	0.01
92	chromium	7440-47-3			
93	chrysene	218-01-9	1.03	0.31	0.13
94	cis-2-butene	590-18-1			
95	Cl2 (a)	7782-50-5	0.00282	0.2	0.001
96	cobalt	7440-48-4	0.00121	0.8	0.001
97	copper	7440-50-8	0.000307	0.3	0.001
98	dibenz(a,h)anthracene	53-70-3	1.68	0.31	0.13
99	dibenzo(b,def)chrysene-7,14 dione (c.i. vat yellow 4)	128-66-5			
100	dibutyl phthalate	84-74-2	0.0598	1	0.01
101	dichloroacetonitrile	3018-12-0			
102	dichlorodiflouromethane	75-71-8	0.0119	0.23	0.01
103	dimethyltrisulfide	3658-80-8			
104	diphenylamine	122-39-4	0.054	0.5	0.01
105	ethane	74-84-0			
106	ethanol	64-17-5			
107	ethyl benzene	100-41-4	0.0739	0.97	0.01
108	ethyl chloride	75-00-3	0.00798	0.8	0.01

(Sheet 3 of 5)

Table 15 (Continued)

ID	Chemical	CAS Number	K_p, cm/hr	GI ABS (fraction)	Dermal ABS (fraction)
109	ethylene	74-85-1			
110	fluoranthene	206-44-0	0.513	0.31	0.13
111	fluorene	86-73-7	0.171	0.5	0.13
112	formaldehyde	50-00-0	0.00221	0.8	0.01
113	furan	110-00-9	0.00655	0.8	0.01
114	HCl	7647-01-0	0.0028	0.2	0.001
115	heptanal	111-71-7			
116	hexachlorobenzene	118-74-1	0.408	0.5	0.01
117	hexachlorobutadiene	87-68-3	0.121	0.5	0.01
118	hexachlorocyclopentadiene	77-47-4	0.156	0.5	0.01
119	hexachloroethane	67-72-1	0.0596	0.5	0.01
120	hexanal	66-25-1			
121	hexane	110-54-3	0.334	0.8	0.01
122	HMX	2691-41-0	0.000114	0.15	0.01
123	hydrogen cyanide	74-90-8	0.000866	0.17	0.001
124	i-butane (isobutane)	75-28-5			
125	i-butene (isobutene/e-butylene)	115-11-7			
126	indeno(1,2,3-cd)pyrene	193-39-5	2.23	0.31	0.13
127	isothiocyanatomethane	556-61-6			
128	lead	7439-92-1	0.000342	0.15	0.001
129	xylene (mixed isomers)	1330-20-7	0.0704	0.92	0.01
130	m-xylene (meta-xylene)	108-38-3	0.0802	0.8	0.01
131	p-xylene (para-xylene)	106-42-3	0.0739	0.8	0.01
132	magnesium	7439-95-4	0.000518	0.2	0.001
133	manganese	7439-96-5	0.00128	0.04	0.001
134	m-dichlorobenzene	541-73-1	0.0775	0.8	0.01
135	mercury	7439-97-6	0.000314	0.07	0.001
136	methacrolein	78-85-3			
137	methane	74-82-8			
138	methylene chloride	75-09-2	0.00446	0.95	0.01
139	methylnitrite	624-91-9			
140	methyl-t-butylether (MTBE)	1634-04-4	0.00257	0.8	0.01
141	methyl-vinyl ketone	78-94-4			
142	naphthalene	91-20-3	0.0694	0.8	0.13
143	n-butane	106-97-8			
144	n-decane	124-18-5			
145	NH3 (ammonia)	7664-41-7	0.000157	0.2	0.001
146	nickel	7440-02-0	0.000329	0.27	0.001
147	nitric acid	7697-37-2			
148	nitrobenzene	98-95-3	0.00696	0.97	0.01
149	nitrogen oxide (NOx)	10102-44-0	0.000384	0.2	0.001
150	nitroglycerine	55-63-0			
151	nitromethane	75-52-5			
152	nonanal	124-19-6			
153	OCDD (1,2,3,4,6,7,8,9-OCDD)	3268-87-9	16.5	0.5	0.03
154	octanal	124-13-0			
155	o-dichlorobenzene	95-50-1	0.0659	0.8	0.01

(Sheet 4 of 5)

Table 15 (Concluded)

ID	Chemical	CAS Number	K_p, cm/hr	GI ABS (fraction)	Dermal ABS (fraction)
156	o-methoxy-phenyl-azo-b-naphthol (oil red g)	1229-55-6			
157	o-xylene (ortho-xylene)	95-47-6	0.0704	0.8	0.01
158	particulate cyanide	57-12-5			
159	p-dichlorobenzene (para-dichlorobenzene)	106-46-7	0.0669	0.9	0.01
160	pentaerythritoltetranitrate (PETN)	78-11-5			
161	perchloroethylene	127-18-4	0.0481	1	0.01
162	phenanthrene	85-01-8	0.229	0.73	0.01
163	phenol	108-95-2	0.00553	0.9	0.01
164	phenylacetylene (ethynyl benzene)	536-74-3			
165	phosphorus	7723-14-0	0.000759	0.2	0.001
166	propanal	123-38-6			
167	propane	74-98-6			
168	propylene	115-07-1			
169	propyne	74-99-7			
170	pyrene	129-00-0	0.324	0.31	0.13
171	RDX	121-82-4	0.000349	1	0.01
172	selenium	7782-49-2	0.000903	0.44	0.001
173	silver	7440-22-4	0.000609	0.18	0.001
174	styrene (vinyl benzene)	100-42-5	0.0548	0.8	0.01
175	sulfur dioxide (SO2)	7446-09-5			
176	sulfuric acid	7664-93-9			
177	tetryl (2,4,6-trinitrophenylmethylnitramine)	479-45-8	0.000496	0.5	0.01
178	thallium	7440-28-0	0.000157	0.15	0.001
179	thiophene	110-02-1			
180	toluene	108-88-3	0.0453	0.8	0.01
181	trans-2-butenal	123-73-9	0.0019	0.5	0.01
182	trans-2-butene	624-64-6			
183	trans-2-pentene	646-04-8			
184	trans-3-penten-2-one	625-33-2			
185	trichloroethylene (TCE)	79-01-6	0.0157	0.15	0.01
186	trichloroflouromethane	75-69-4	0.0173	0.23	0.01
187	vinylidenechloride	75-35-4	0.0159	1	0.01
188	zinc	7440-66-6	0.000342	0.2	0.001

Note: Values of 0.8, 0.5, and 0.2 for GI ABS and 0.01 and 0.001 for dermal ABS are most like default values.

Statistical Summary

Number of available data values	111	111	111
Number of not available data values	77	77	77
Percent of AVAILABLE DATA VALues	60	60	60

(Sheet 5 of 5)

Data Gaps, Conclusions, and Recommendations

For now, due primarily to USEPA recommendations, Equation 15 is recommended for estimating K_p for chemicals that do not have measured values. Future studies should be conducted to evaluate other empirical equations, such as

Equation 16, and other types of models, such as the anatomically based, physical models.

USEPA provides GI absorption values for a limited number of chemicals. USEPA recommends default GI ABS values of 0.8 for volatile organics, 0.5 for semivolatile organics, and 0.2 for inorganic chemicals when measured values are not available. It appears that GI ABS should receive greater attention since values are not available for many compounds. For now, USEPA-recommended default values can be used in the absence of measured values.

USEPA has provided an empirical equation (Equation 17) to calculate the dermal ABS. However, this equation requires several parameters that must be measured, estimated, or computed, making the use of this equation problematic. The ARAMS/FRAMES and RAIS Databases provide some limited data for the Range chemicals, which will be added to the Range Database. USEPA (1992a) recommends using 0.001 for inorganics and 0.01 for organics as default values for dermal ABS when values are not available otherwise. However, in some cases, the default values may overestimate dermal exposure. Thus, further study for this parameter may be justified.

Table 16 provides a summary of recommended sources for each of the human exposure parameters for use in the Range Database. The RAIS Database has data for 111 (60 percent) of the chemicals in the list (Table 15), but many of these values are the USEPA recommended default values. The ARAMS/ FRAMES Database has data for 39 to 67 (10 to 36 percent) of the chemicals (Table 14). The majority of missing data in the ARAMS/FRAMES Database is for dermal absorption fraction. USEPA has provided default values for GI ABS and dermal ABS. Of the three exposure parameters, the dermal absorption fraction should probably receive the most attention in future research.

Table 16
Recommended Sources for Human Exposure Parameters

Parameter	Unit	Source		
		Equation Number	Tables	USEPA Defaults
Aqueous skin permeability	cm/hr	15	11, 14, 15	
GI absorption fraction (GI ABS)	fraction		12, 14, 15	0.8 vol. organic 0.5 semi vol. organic 0.2 inorganic
Dermal absorption fraction from soil	fraction		13, 14, 15	0.001 inorganic 0.01 organic

5 Food Transfer Factors

Introduction

Transfer factors, also known as concentration ratios or bioaccumulation factors, are the ratio of the concentration of an element in an organism of interest, such as plants and food products, to the concentration in the source medium, such as soil (for plants), plant forage (for animals), or water (for fish, crustaceans, mollusks, and aquatic plants). The transfer factor applies to long-term, chronic exposure of plants and animals and is ideally measured at equilibrium (steady-state).

Measurements are a preferred source of data for food transfer factors. However, such measurements are expensive and often limited. Estimating food transfer factors using mathematical models and physicochemical properties has received considerable consideration in the literature.

Bioaccumulation is the process that causes an increased chemical concentration in an organism as a result of chemical uptake through all possible routes of chemical exposure. Bioaccumulation is a combination of chemical bioconcentration and biomagnification (Gobas and Morrison 2000). Bioconcentration is the increase of the concentration in an organism as the result of diffusive mass transfer of a contaminant in the environment. Biomagnification is the increase of the concentration in an organism as a result of consumption of contaminated food (Jager and Hamers 1997; Gobas and Morrison 2000). Bioaccumulation and bioconcentration are usually expressed in the form of a bioaccumulation factor (BAF) or bioconcentration factor (BCF), respectively, which is the ratio of the chemical concentration in the organism to that in the environment.

A compound's BCF is the most commonly used indicator of its tendency to accumulate in aquatic organisms from the surrounding medium. Because it is expensive to measure, the BCF is generally estimated from physicochemical properties such as K_{ow}. There are two general approaches for quantifying bioaccumulation, empirical and mechanistic (MacKay and Fraser 2000). From an empirical approach, the BAF can be deduced from the concentration in the organism and a measured experimental concentration. The mechanistic approach applies a mass balance model in which the various uptake and loss processes are quantified. Such models need more data about the chemical and the organism. Empirical models are descriptive, where mechanistic models are more

explanatory. The mechanistic approach can involve either a steady-state or a dynamic model. Mechanistic models are based on one or more mathematical equations. In contrast, an empirical model is based on a statistical summary of observational data. The empirical modeler often uses the observational data as a guide in the selection of the model specification and to provide estimates of parameters. More information about the mechanisms and models of bioaccumulation can be found in Jager and Hamers (1997).

The currently used regression equations (empirical approach) were usually developed from small data sets and should be used with caution for the large range of chemical substances now subject to review. To develop an improved method, more measured BCFs and other key experimental details for chemicals are needed. This chapter describes available models that may be used to estimate food transfer factors.

Methods

The literature search was carried out using Internet Web pages, published journal articles such as *Environmental Science and Technology, Chemosphere, Environmental Toxicology and Chemistry, Environmental Pollution, SAR and QSAR in Environmental Research*, and USEPA reports. Available databases, such as RAIS (http://risk.lsd.ornl.gov/cgi-bin/tox/TOX_select?select=csfand) and the ARAMS/FRAMS (http://el.erdc.usace.army.mil/arams/) constituent database, were also searched for data on these parameters.

Bioaccumulation in Fish

Bioconcentration is defined as the result of the uptake, distribution, and elimination of a chemical in a fish due to water-borne exposure (Barron 1990). The bioconcentration factor for fish (BCF_{fish}) is the ratio of the chemical concentration in fish to the chemical concentration in the water column where the fish is exposed. The BCF_{fish} accounts for uptake of chemicals in fish by water passing across the gills. The methods summarized in this section apply to freshwater fish in general and do not distinguish types, such as finfish and shellfish.

Bioaccumulation includes all routes of exposure, and biomagnification deals with accumulation via food chains. The bioaccumulation factor for fish (BAF_{fish}) is the ratio of the chemical concentration in the fish to the concentration in the water body where the fish is exposed. However, the BAF accounts for uptake of chemicals by fish from water and sediments passing across the gills and from consumption of various foods including plankton, daphnids, and other fish. The relationship between BAF_{fish} and BCF_{fish} is given as:

$$BAF_{fish} = BCF_{fish} \times FCM \tag{18}$$

where FCM is the food chain multiplier, either obtained from Table 17 (USEPA 1995a, 1995c) or from appropriate measured field data.

Table 17
Food-Chain Multipliers for Tropic Levels 2, 3, and 4

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4	Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
4.0	1.00	1.23	1.07	6.6	1.00	12.9	23.8
4.1	1.00	1.29	1.09	6.7	1.00	13.2	24.4
4.2	1.00	1.36	1.13	6.8	1.00	13.3	24.7
4.3	1.00	1.45	1.17	6.9	1.00	13.3	24.7
4.4	1.00	1.56	1.23	7.0	1.00	13.2	24.3
4.5	1.00	1.70	1.32	7.1	1.00	13.1	23.6
4.6	1.00	1.87	1.44	7.2	1.00	12.8	22.5
4.7	1.00	2.08	1.60	7.3	1.00	12.5	21.2
4.8	1.00	2.33	1.82	7.4	1.00	12.0	19.5
4.9	1.00	2.64	2.12	7.5	1.00	11.5	17.6
5.0	1.00	3.00	2.51	7.6	1.00	10.8	15.5
5.1	1.00	3.43	3.02	7.7	1.00	10.1	13.3
5.2	1.00	3.93	3.68	7.8	1.00	9.31	11.2
5.3	1.00	4.50	4.49	7.9	1.00	8.46	9.11
5.4	1.00	5.14	5.48	8.0	1.00	7.60	7.23
5.5	1.00	5.85	6.65	8.1	1.00	6.73	5.58
5.6	1.00	6.60	8.01	8.2	1.00	5.88	4.19
5.7	1.00	7.40	9.54	8.3	1.00	5.07	3.07
5.8	1.00	8.21	11.2	8.4	1.00	4.33	2.20
5.9	1.00	9.01	13.0	8.5	1.00	3.65	1.54
6.0	1.00	9.79	14.9	8.6	1.00	3.05	1.06
6.1	1.00	10.5	16.7	8.7	1.00	2.52	0.721
6.2	1.00	11.2	18.5	8.8	1.00	2.08	0.483
6.3	1.00	11.7	20.1	8.9	1.00	1.70	0.320
6.4	1.00	12.2	21.6	9.0	1.00	1.38	0.210
6.5	1.00	12.6	22.8				

Source: USEPA (1995a, 1995c).

Empirical BCF models

Devillers et al. (1996) studied several published correlations for bioconcentration factor and recommended the equation reported by Bintein et al. (1993). This model relates BCF_{fish} (L/kg fish tissue) to K_{ow},

$$\log BCF_{fish} = 0.91 \times \log K_{ow} - 1.975 \log (6.8E-7 \times K_{ow} + 1) - 0.786 \quad (19)$$

BCF data show a drop in BCF at high K_{ow} values ($\log K_{ow} > 6$). The fall above $\log K_{ow}$ of 6 is presumably a result of reduced bioavailability. Equation 19 gives such a drop, where the bioconcentration reaches a maximum and then falls above $\log K_{ow}$ of 6. Devillers et al. (1998) found that the Bintein et al. (1993) gives good simulation results and that the model presents a large $\log K_{ow}$ domain of application.

USEPA (1988) recommends the following equation by Lyman et al. (1982b) and Veith et al. (1980) for BCF_{fish} for organic chemicals,

$$\log BCF_{fish} = -0.23 + 0.76 \log K_{ow} \quad (20)$$

Note that the above equations are used to calculate BCF_{fish} values only for organic compounds. Both Equations 19 and 20 are also available in the ARAMS/FRAMES constituent database editor for estimating BCF_{fish}. Estimating

BCF values for inorganic chemicals is more problematic. There is no handy estimation equation. Values must be searched on a chemical-by-chemical basis. Table 18 is an example of recommended values obtained from the California Environmental Protection Agency (2000) that has BCF values for metals taken up in fish.

Table 18
Summary of Recommended Default Fish BCFs

Chemical	BCF
4, 4-methylene dianiline	11.1
arsenic	4
cadmium	366
chromium	2
dioxins and furans	19,000
hexachlorocylcohexanes	456
hexachlorobenzene	13,130
lead	155
mercury (inorganic)	5,000
PAH as bezo[a]pyrene	583
polychlorinated biphenyls	99,667
diethylhexlphthalate	483.1

Source: California EPA (2000, Appendix H).

The use of empirical correlations to describe bioconcentration phenomena in aquatic organisms using physiochemical properties of the chemical was first reported by Neely et al. (1974). Using rainbow trout, the uptake and clearance rates of a variety of chemicals were measured experimentally in the laboratory. Veith et al. (1979) extended this approach to more chemicals and obtained a two-parameter relationship for fathead minnows. Mackay (1982) also examined the same data and argued that the slope of 0.85 was not significantly different from 1.0 and that the simpler one-parameter relationship applies. Many of the empirical relationships tend to break down when dealing with highly hydrophobic chemicals (Bintein et al. 1993).

According to Mackay and Fraser (2000) and Gobas and Morrison (2000), it is necessary to specify that the BCF be deduced from the dissolved rather than the total aqueous concentration. If the total concentration is used, the BCF will depend on sorption conditions in the water, which are unrelated to uptake and clearance by the organism. An unnecessary variability is introduced into the interpretation of BCFs by using the total concentration in water. The use of the freely dissolved concentration in water is particularly important for highly hydrophobic chemicals (log $K_{ow} > 5$), which exhibit a high tendency to associate with organic matter in the water.

Meylan et al. (1999) have proposed a more detailed method of predicting BCFs from K_{ow}. It is believed that the discrepancies that exist between the predicted BCFs from the derived empirical relationships and those observed in the environment are partly due to the relatively small data sets used in the past studies. Meylan et al. (1999) analyzed and grouped 694 chemicals and obtained several correlations for nonionic and ionic compounds, including correction

factors for the BCF estimation of several compound classes. For both groups of compounds, the proposed equations resulted in a higher correlation coefficient than for equations established with other empirical models, such as Veith et al. (1979) and Bintein et al. (1993). The equations of Meylan have the advantages that they are based on a large data set with a wide range of K_{ow}, they allow for metabolic conversion, and they can be used for ionic compounds. The equations also predict the observed reduction in BCF for nonionic compounds when the log K_{ow} exceeds 7.

Empirical models may calculate inaccurate values because of uncertainty about the K_{ow} for a compound. The K_{ow} is also pH dependent for ionizing compounds creating further uncertainty. There is no mechanistic treatment of bioavailability. For screening purposes, the Bintein et al. (1993) model (Equation 19) may be preferred and was used for the organic chemicals in the Range Database.

More recently, in two studies Lu et al. (1999, 2000) investigated the molecular connectivity index (MCI) method for a wide range of nonionic organic substances. The MCI is a nonempirical parameter that is derived from the molecular structure only and has been demonstrated correlating to many physiochemical properties including water solubility, K_{ow}, and K_{oc}. Although the MCI is a nonempirical parameter, the relationship that correlates it to the BCF is an empirical one. The underlying idea of this method is to count the bonds of the hydrogen-suppressed molecular skeleton and to derive an index from them. Hence, the index is based on the structure of the molecule and has been shown to correlate with the size, number of branches, volume, and surface area of a molecule. The index correlates to experimentally determined biotransfer factors and can serve as a surrogate for a K_{ow}-based correlation. MCI could be described as more flexible because it can be computed directly from the structure of organic compounds (Lu et al. 1999, 2000). MCI is also able to reduce uncertainties with regard to the K_{ow} value. MCI was found to be a good descriptor of BCF for nonpolar compounds, but not for polar ones (Lu et al. 2000). The main disadvantage of the MCI approach is that this method is not properly validated and not yet broadly applicable. Further, the MCI is a calculated variable for which more substance information is needed to calculate other variables (i.e. number of atoms and branches of a molecule or molecular surface area). Therefore, MCI is a relatively complicated method compared to the log K_{ow} approach. The MCI approach should be investigated more closely in a future effort.

The above empirical models for fish were developed for freshwater fish. Therefore, the existing models must be used with care for marine fish. The bulk of the consumed fish is retrieved from the marine water environment and not from the freshwater environment. This contradiction should be examined further in the future.

Mechanistic models

During the last decade, several authors have developed more complex mechanistic models that integrate bioconcentration, biomagnification, growth, and elimination. Gobas and Morrison (2000) distinguish three types of mechanistic models: kinetic models, physiological models (i.e. PBPK), and foodweb bioaccumulation models.

Jager and Hamers (1997) investigated a kinetic model suitable for considering bioconcentration, metabolism, and growth. The model describes the partitioning between fish and water and is based on the volume fractions of water and lipids in the fish. Other constituents of the fish are assumed to have no affinity for the chemical. Metabolism and growth dilution can be important for very hydrophobic chemicals and are described by kinetic rate constants. The model also uses rate constants for diffusive uptake and elimination, which can be estimated according to Sijm and Linde (1995).

Thomann (1989) and Gobas (1993) have developed physiologically based kinetic models, including rate constants for chemical uptake and elimination based on physiological parameters (i.e. gill ventilation, feeding, and chemical assimilation). Both models are used widely and have been tested against field data. The model predictions are generally within a factor of two to three of the observation made in the field, which can be regarded as acceptable (Gobas and Morrison 2000). The physiologically based kinetic model of Thomann (1989) and Thomann et al. (1992), which considers biomagnification and the organism's rank in the food chain, explained the increasing error in predicting the BCF with an increasing degree of lipophilicity. The K_{ow} is used to describe the tendency of chemicals to partition into the lipid compartments of the organisms. The model consists of five biological compartments, including benthic organisms. Four contaminant exposure routes are considered: ingestion of particulates and phytoplankton and ventilation in overlying and interstitial waters. For the simple lipid partitioning of a chemical into an organism, the growth of the organism is recognized by the model. For generic growth rates across a simple food chain, the model calculations indicate that field log BCF values could be expected to be at a maximum of about 5.5 at a log K_{ow} of about 6. Subsequent increases in K_{ow} do not result in proportional increases in BCF because of growth and transfer efficiency effects. After a value of approximately 6.5, the BCF begins to decline. Below log K_{ow} of 5, decreased uptake and increased excretion prevent food chain buildup.

The steady-state food web bioaccumulation model of Gobas (1993) was developed to estimate bioconcentration factors, biomagnification factors, and bioaccumulation factors as well as concentrations and fugacities in phytoplankton, zooplankton, benthic invertebrates, and fish species in water and sediments. The model uses rate constants to describe the considered processes for organisms of a defined food web. The model estimates the intake of chemicals from the gills and the diet and the rate of elimination via gills, feces, growth, and metabolic transformation. The excretion rate constant is set at approximately 25 percent of the dietary uptake rate constant and bioavailability is also considered. The model can be applied to many aquatic food webs and uses a

relatively small set of input parameters. The uptake efficiency remains constant as log K_{ow} increases, until a value of about 6 or 7 is reached after which the uptake efficiency decreases. The model was applied to a Lake Ontario food web and yielded satisfactory results, despite the relatively small number of required model input parameters (Mackay and Fraser 2000). The 95 percent confidence interval of the ratio of observed and predicted concentrations of persistent organic chemicals was within a factor of two to three. The USEPA reviewed the model in 1994 and applied it in its Great Lakes Water Quality Initiative (Gobas and Morrison 2000). The advantage of this relatively simple model is the consideration of processes, including feeding interactions that may improve the results. The weakness of the Thomann and Gobas models is that they treat only a single organism per trophic level (Mackay and Fraser 2000). Due to the required database, the models are not considered practical for the screening stage of a risk assessment. The complexity of the mechanistic models makes them impractical for use in estimating BCF values for the Range Database chemicals.

Recommendations for fish models

There are several accepted relationships for calculating BCF from log K_{ow} values for nonpolar, hydrophobic organic chemicals that have been and continue to be used in regulatory applications. According to Devillers et al. (1996), these equations yield equivalent results for organic chemicals with log K_{ow} less than 6. But, for chemicals with log K_{ow} values higher than 6, the bilinear model of Bintein et al. (1993) (Equation 19) is recommended by Devillers et al. (1996). For the chemicals in the list where experimental results were available, AME was calculated using both Equations 19 and 20 and results are shown in Table 19. Equations 19 and 20 resulted in about the same AME for the data in Table 19. However, since Equation 19 allows a decrease in BCF for log $K_{ow} > 6$, it was used for the Range Database.

Table 19
A Comparison of BCF Values from Equations 18 and 19 and Experimental Data

Chemical	CAS Number	Log K_{ow}	log BCF (Eq. 19)	Experimental log BCF	Log BCF (Eq. 20)
1,2-dichlorethane	107-06-2	1.48	0.56	0.30	0.89
1,3-dinitrobenzene	99-65-0	1.62	0.69	1.87	1.00
2,4-dinitrotoluene (DNT; 2,4-DNT)	121-14-2	2.00	1.03	2.31	1.29
2,6-dinitrotoluene (2,6-DNT)	606-20-2	2.10	1.12	2.44	1.37
2-nitrotoluene (ONT)	88-72-2	2.30	1.31	2.28	1.52
acenaphthene	83-32-9	3.92	2.78	2.59	2.75
acrolein	107-02-8	0.90	0.03	2.54	0.45
benzo(a)pyrene	50-32-8	5.97	4.23	3.51	4.31
fluorene	86-73-7	4.20	3.03	3.35	2.96
hexachlorobenzene	118-74-1	5.23	3.88	5.62	3.75
hexachloroethane	67-72-1	4.60	3.38	3.08	3.27
naphthalene	91-20-3	3.23	2.15	2.49	2.23
nitrobenzene	98-95-3	1.85	0.90	1.47	1.18
phenol	108-95-2	1.46	0.54	1.24	0.88
pyrene	129-00-0	4.88	3.61	3.68	3.48
AME (log BCF) (percent)			39.3		39.6
Average bias (log BCF)			-0.64		-0.50

Feed to Animal Transfer Factors

This section presents feed to animal transfer factors for beef and milk, pork, poultry, and eggs. The biotransfer factor for animals is the ratio of chemical concentration in fresh weight (FW) animal tissue (g/kg FW) to the daily intake rate of chemical by the animal (g/day).

Biotransfer factors for beef and milk

For organics, empirical correlation equations as a function of K_{ow} have been developed to calculate transfer factors for beef (Ba_{beef}, days/kg FW) and milk (Ba_{milk}, days/kg FW). In the ARAMS/FRAMES Database, Ba_{milk} has units of days per liter (1 day/L = 1.03 days/kg). Travis and Arms (1988) introduced a log-linear geometric mean regression equation based on experimentally derived bioaccumulation factors and log K_{ow} for fresh meat and milk. The bioaccumulation factor for meat was derived from data on 36 organic compounds, with a log K_{ow} range of 1.34 to 6.47. The bioaccumulation factor for milk was derived from data on 28 organic compounds, with a log K_{ow} range of 2.81 to 6.89. The organic compounds included compounds from DDT, pesticide, polychlorinated dibenzo-p-dioxin (PCDD), and PCB classes. The Travis and Arms (1988) correlation equations are

$$\log Ba_{beef} = -7.6 + \log K_{ow} \tag{21}$$

$$\log Ba_{milk} = -8.1 + \log K_{ow} \tag{22}$$

McLachlan et al. (1990) conducted studies on lactating cows and found for dioxin-like compounds the above equations overestimated Ba_{beef} and Ba_{milk} values.

For inorganic constituents, USEPA recommends Ba_{beef} and Ba_{milk} values from Baes et al. (1984). The data from Baes et al. (1984) are shown in Figures 2 and 3. For the Range Database, all values given in Figures 2 and 3 are used. For cadmium, selenium, and zinc, USEPA (1992b) recommends values of 1.20E-04, 2.27E-03, and 9.0E-05 (days/kg FW) for Ba_{beef}, and, 6.50E-06, 5.86E-03, and 3.25E-05 (days/kg FW) for Ba_{milk}, respectively.

Evaluation of meat and milk models. The main criticisms of the Travis and Arms (1988) models are: they do not predict concentrations accurately for high log K_{ow} values; they fail to accurately predict concentrations for rapidly metabolizing chemicals; they were derived based on data that were not at steady-state; and they underestimate beef biotransfer factors (BTF) because they include data for lactating cows and assume constant chemical intake rates for beef cattle (Birak et al. 2001). Predictive bioaccumulation models inherently assumed a steady-state condition between chemical intake and elimination. This assumption oversimplifies the behavior or lactating status of a cow. Sufficient uptake time is necessary for reaching steady state. Some chemicals never reach a steady-state condition within the lifetime of an animal or human (e.g. OCDD). For about

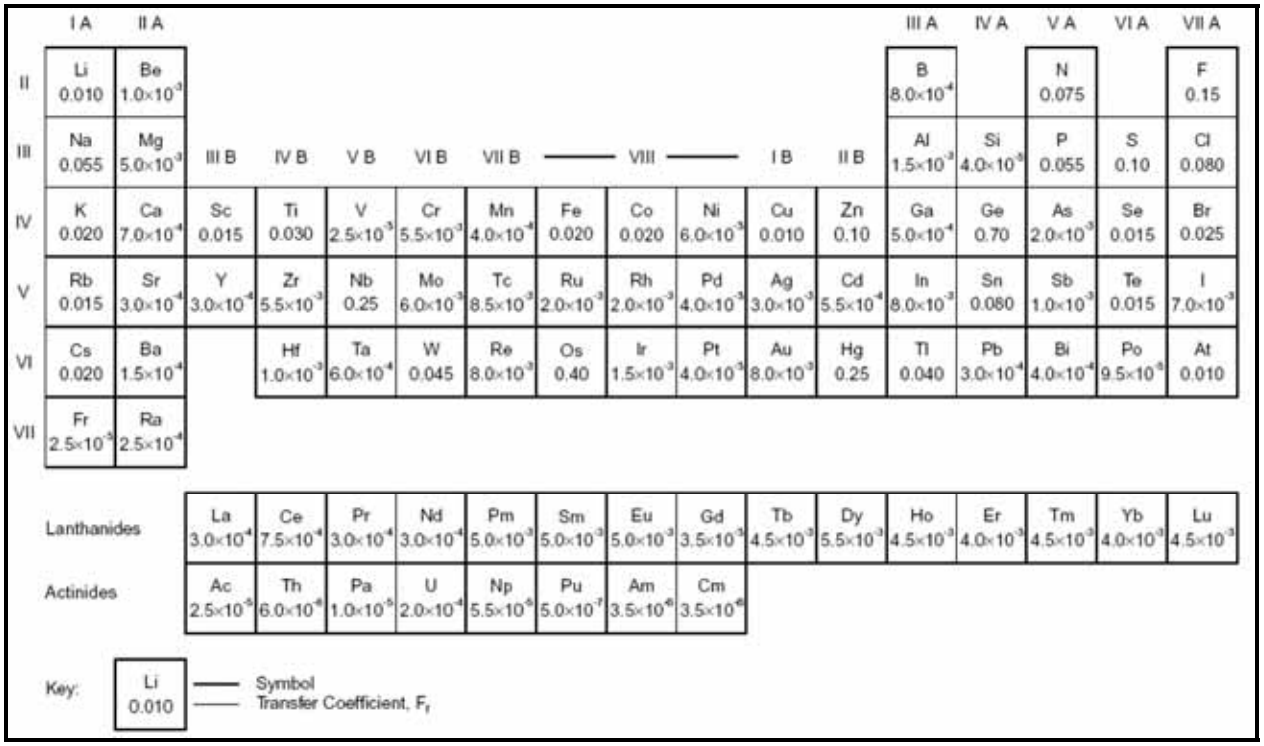


Figure 2. Values of the ingestion-to-beef transfer coefficient, F_r (days/kg) (Source: Baes et al. 1984)

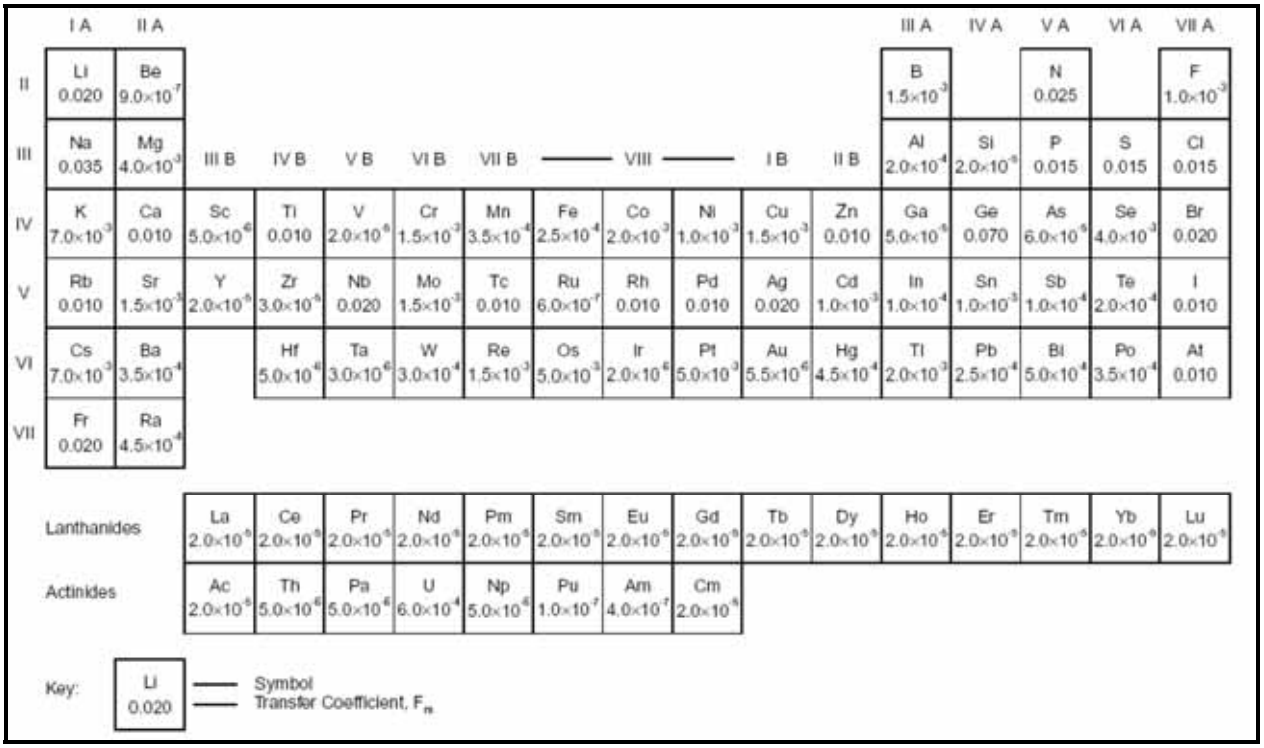


Figure 3. Values of the ingestion-to-milk transfer coefficient, F_m (days/kg) (Source: Baes et al. 1984)

70 percent of the meat bioaccumulation factors, Travis and Arms (1988) used data based on concentrations in nonlactating cattle (Birak et al. 2001). An analysis has not yet been conducted to determine if there is a significant difference in the concentrations for the same chemical between lactating and non-lactating cattle.

Birak et al. (2001) evaluated the bioconcentration algorithms of Travis and Arms (1988), conducted an analysis to validate the Travis and Arms approach, and expanded their data for deriving updated regression equations. The Birak et al. (2001) analysis utilized a well-defined set of criteria for data collection and analysis to derive BTFs from K_{ow} values. Birak et al. considered log K_{ow} from 1.5 to 8.8 for milk and from 1.4 to 8.8 for beef. The results based on additional data are consistent with more recent literature, which has shown decreasing BTFs for high log K_{ow} compounds. The Travis and Arms regressions may greatly overestimate beef and milk concentrations for compounds with a log $K_{ow} > 6.5$. This was also described by McLachlan (1994) and Thomas et al. (1998), demonstrating that the concentrations in milk and beef decrease with increasing log K_{ow} for log K_{ow} values higher than 6. The Travis and Arms equations predict that concentration continue to increase with increasing log K_{ow}. In addition, the data suggest that concentrations may be underestimated for compounds with lower log K_{ow} values. The advantage of the expanded database is that it can be used for chemicals with a large log K_{ow} range. Nevertheless, the expanded database did not improve the regression equations developed by Travis and Arms, and the variability in BTFs is even higher than the variability for the Travis and Arms data alone. Another disadvantage of the Travis and Arms (1988) model is that the sources of the K_{ow} values that were used for the regression equations are not stated.

The regressions of Travis and Arms (1988) represent a simplification of chemical uptake and excretion and ignore important toxicokinetic processes, such as metabolism (Sweetman et al. 1999). Metabolism is usually attributed to enzyme-mediated degradation in the liver and has been shown to be an important loss for certain chemicals. However, metabolism seems to be adequately modeled by first-order kinetics and can, therefore, be integrated well into a steady-state model.

A study of Jager et al. (1997) has indicated there is considerable uncertainty of the Travis and Arms (1988) regression for the biotransfer to meat and milk, with an uncertainty factor of 64 and 36, respectively. The model for meat provides good results for the lower chlorinated dioxins (within one log unit), but higher dioxins are overestimated. PCBs are underestimated by up to a factor of 100. The model for milk seems to overestimate the concentrations. Overall, the models provide conservative results, but in some situations, significant underestimation may occur.

Alternative models for meat and milk. Dowdy et al. (1996) developed molecular connectivity indices (MCI) to predict the biotransfer factor of organic compounds in meat and milk. The MCI is a nonempirical parameter that is derived from the molecular structure. Dowdy et al. compared the predicted uptake of the MCI approach with experimental values and relative to the

K_{ow} approach. The data set, mainly pesticides, contained 35 compounds for meat and 34 compounds for milk. For a known, constant K_{ow}, Travis and Arms (1988) delivers better results than the MCI approach. For an uncertain K_{ow}, the inaccuracy of the K_{ow}-based approach is more than that of the MCI-based method, and the coefficient of variation is four times larger. The MCI method results in better estimations for dioxins and in poorer estimations for PCBs. However, the MCI method always leads to lower concentrations in meat and milk. Compared to the K_{ow} approach, MCI does not have as much inherent uncertainty due to measurement and estimation errors. MCI has a large potential for reliably estimating the BCF of new substances and has few limitations in its use. However, MCI is a relatively complicated method compared to the log K_{ow} approach, for which more substance information is needed to calculate the value and the polar correction. The data set of Dowdy et al. (1996) used a limited number of high K_{ow} compounds (Birak et al. 2001). The main disadvantages of MCI are that validation of this method is limited and the method is not yet broadly applicable.

Conclusions of meat and milk models. The bioaccumulation estimation into meat and milk may include large uncertainties. The relation of Travis and Arms may be improved by using reliable experimental log K_{ow} values. Further investigations are needed to determine if the models of Dowdy et al. (1996) or McLachlan (1994) are a better alternative. The Travis and Arms equations predict an increase in the concentrations in milk and meat with increasing log K_{ow}. This may greatly overestimate the concentration in milk and meat because, for high log K_{ow} compounds (log $K_{ow} > 6$), the bioaccumulation factors have been found to decrease. The fat content of meat used for the Travis and Arms (1988) correlation is rather high. All milk products are represented by milk, which is not valid for the much fattier milk products such as cheese and butter. Perhaps it is better to relate concentrations in meat and milk to fat content.

Until another, more reliable method is provided, the Travis and Arms (1988) equations will be used to estimate meat and milk BTFs for organic chemicals in the Range Database. For inorganics, Ba_{beef} and Ba_{milk} values may be obtained from Baes et al. (1984) (see Figures 2 and 3).

Biotransfer factors for pork

For organics (except PCDDs and polychlorinated dibenzofuran (PCDFs)), Ba_{pork} values can be derived from Ba_{beef} (biotransfer for beef) values assuming that pork is 23 percent fat and beef is 19 percent fat (USEPA 1998). Therefore, Ba_{pork} values can be calculated by multiplying Ba_{beef} values by their fat content ratio of 1.2 (i.e., 23/19). This is limited by the assumptions that (1) chemicals bioconcentrate in the fat tissues, and (2) there is minimal effect from differences in metabolism and feeding characteristics between beef cattle and pigs. The equation for pork biotransfer factors is

$$Ba_{pork} = 1.2 \times Ba_{beef}$$

or (23)

$$\log Ba_{pork} = \log 1.2 + \log Ba_{beef} = \log 1.2 - 7.6 + \log K_{ow}$$

For metals (except cadmium, selenium, and zinc), no data were available in the literature for Ba_{pork} values. For cadmium, selenium, and zinc, USEPA (1995c) reported values derived by dividing uptake slopes, obtained from USEPA (1992b), by a daily consumption rate of 4.7 kg DW per day for pigs provided in USEPA (1995b). For cadmium, selenium, and zinc, USEPA values for Ba_{pork} are 1.91E-04, 1.88E-01, and 1.28E-04 (days/kg FW), respectively.

Biotransfer factor for chicken and poultry eggs

Biotransfer factor for chicken ($Ba_{chicken}$, day/kg FW) and poultry eggs (Ba_{egg}, day/kg FW) are expressed as the ratio of the chemical concentration in the fresh weight (FW) tissue to the chemical intake from the feed. For organics (except PCDDs and PCDFs), $Ba_{chicken}$ values can be derived from Ba_{beef} values by assuming that chicken is 15 percent fat and beef is 19 percent fat (USEPA 1998). Therefore, $Ba_{chichen}$ values can be calculated by multiplying Ba_{beef} values by their fat content ratio of 0.8 (i.e., 15/19). This calculation is limited by the assumption that (1) chemicals bioconcentrate in the fat tissues, and (2) there is minimal effect from differences in metabolism or feeding characteristics between beef cattle and chickens. The equation for chicken BTF is

$$Ba_{chicken} = 0.8 \times Ba_{beef}$$

or (24)

$$\log Ba_{chicken} = \log\ (0.8) + \log Ba_{beef} = \log\ (0.8) - 7.6 + \log K_{ow}$$

Ba_{eggs} values can be calculated using an equation from CalTOX (McKone 1993) expressed as

$$\log Ba_{egg} = -5.1 + \log K_{ow} \quad (25)$$

$Ba_{chichen}$ and Ba_{egg} values for metals (except cadmium, selenium, and zinc) are not available in the literature. For cadmium, selenium, and zinc, USEPA (1995b) cited *Ba* values that were derived from dividing uptake slopes (g chemical/kg DW tissue)/(g chemical DW feed), obtained from USEPA (1992b), by a daily feed consumption rate of 0.2 kg DW per day for chickens. For cadmium, selenium, and zinc, USEPA values for $Ba_{chichen}$ are 1.06E-01, 1.13E+00, and 8.75E-03 (days/kg FW), respectively. For cadmium, selenium, and zinc, USEPA values for Ba_{egg} are 2.50E-03, 1.13E+00, and 8.75E-03 (days/kg FW), respectively.

Plant Transfer Factors

Because plant bioaccumulation results are usually compared with medium concentrations, the biotransfer factors are generally bioconcentration factors and are estimated for aboveground biomass and belowground or root biomass.

Aboveground bioconcentration factors

The plant-soil bioconcentration factor (*Br*) for aboveground produce accounts for the uptake from soil and subsequent transport of chemicals through the roots to the aboveground plant parts. The value of *Br* for organics is a function of water solubility, which is inversely proportional to K_{ow}.

For organics, Travis and Arms (1988) developed Equation 26 to calculate values for aboveground produce such as fruits and vegetables, protected fruits and vegetables, and forage, silage, and grain. Travis and Arms (1988) developed only one equation for vegetation (fruit and vegetables) and forage, silage, and grain. They did not distinguish between aboveground produce and forage, silage, or grain. Due to lack of literature data, USEPA (1998) recommends the Travis and Arms (1988) correlation equation for calculating *Br* values for both aboveground produce and forage (µg chemical/g DW plant/µg chemical/g DW soil),

$$\log Br = 1.588 - 0.578(\log K_{ow}) \tag{26}$$

The *Br* values for metals are a function of the bioavailability of the compounds in soil. For metals, including nickel, cadmium, selenium, zinc, and arsenic, *Br* values derived from uptake slope factors are provided in USEPA (1992b). Additionally, for inorganic constituents, *Br* values may be obtained from Baes et al. (1984). Baes et al. (1984) described biotransfer factor (on a dry weight basis) from plant-soil uptake for (1) vegetative growth (leaves and stems), *Bv*, and (2) nonvegetative or reproductive growth (fruit, seeds, and tubers), *Br*, (Figures 4 and 5).

Root plant-soil bioconcentration factors

The plant-soil bioconcentration factor for compounds in root vegetables ($B_{rootveg}$) accounts for uptake from soil to the belowground root vegetables or produce. Briggs et al. (1982) studied the root uptake in barley (cereal grass) and developed the following equation for calculating the root concentration factor (RCF) from water ($\frac{\text{µg/g DW plant}}{\text{µg/mL soil water}}$):

$$\log (RCF - 0.82) = 0.77 \log K_{ow} - 1.52 \tag{27}$$

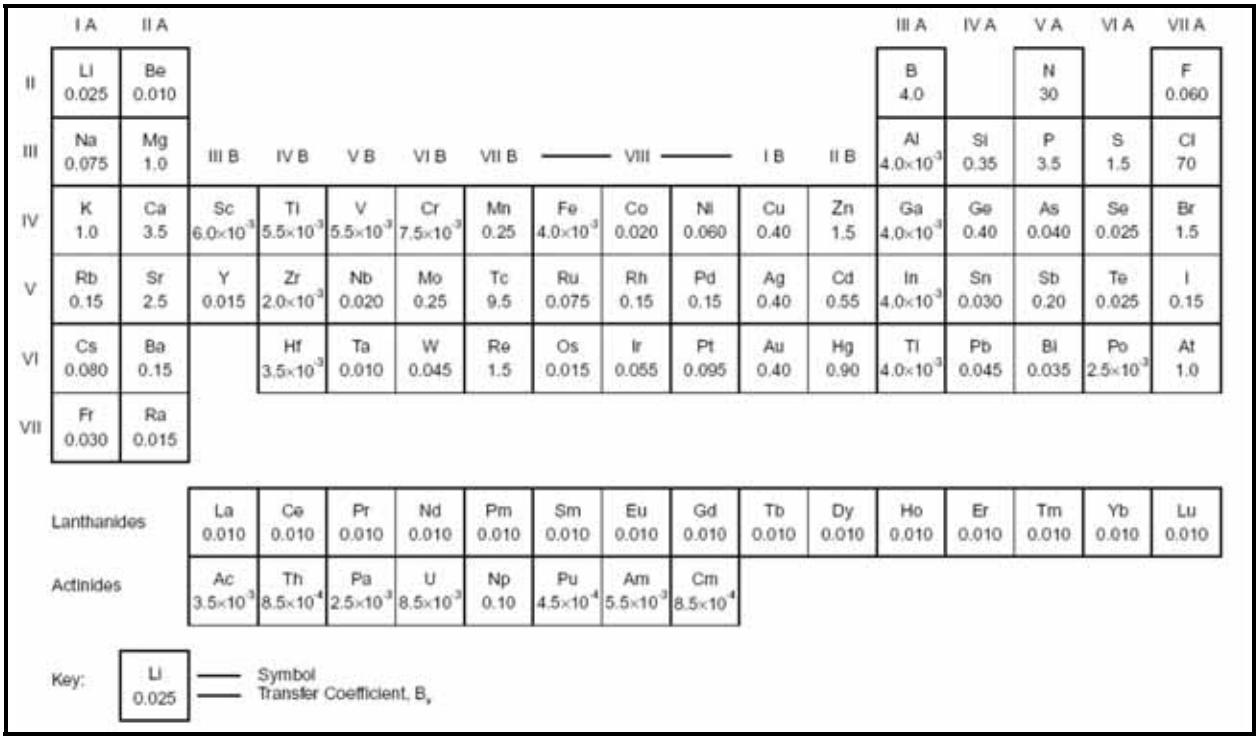


Figure 4. Values of the soil-to-plant bioconcentration factor, *Bv*, for vegetative growth (leaves and stems) (Source: Baes et al. 1984)

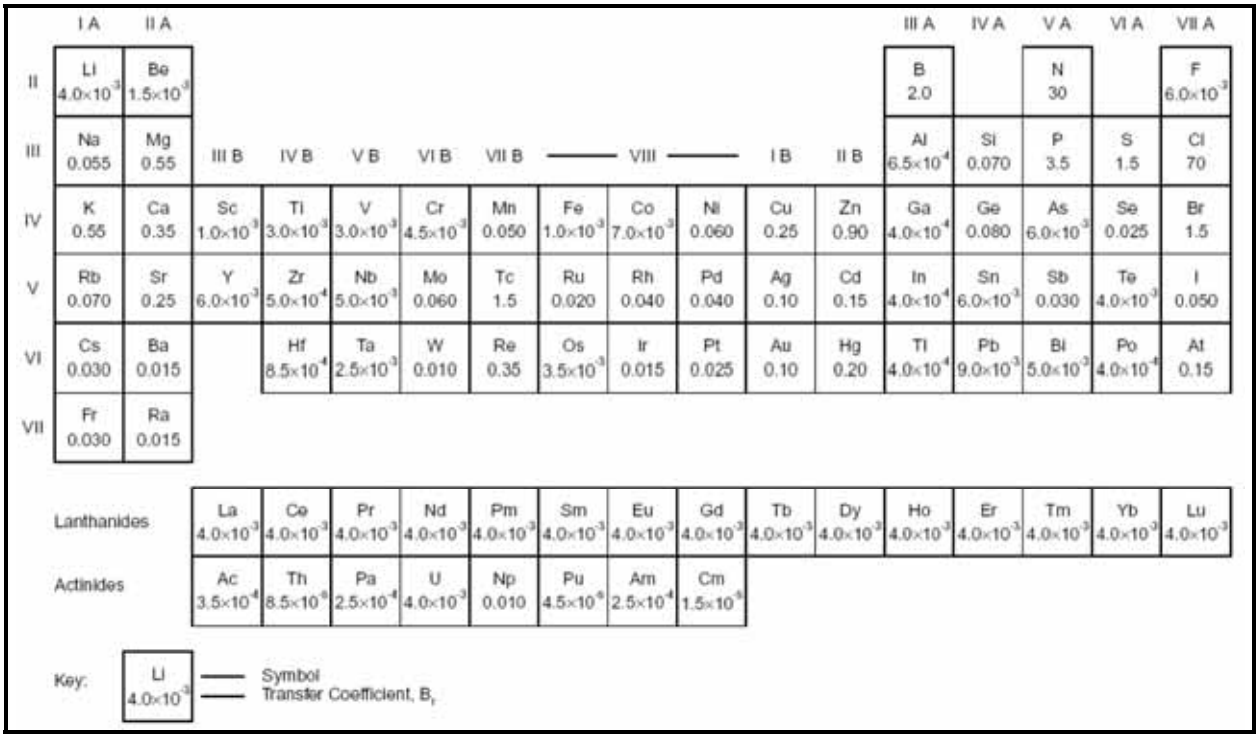


Figure 5. Values of the soil-to-plant bioconcentration factor, *Br*, for nonvegetative growth (fruits, seeds) (Source: Baes et al. 1984)

where

$$RCF = \frac{\text{concentration in roots (FW)}}{\text{concentration in water}}$$

This equation estimates an *RCF* value in fresh weight (FW) units, which then may be converted to dry weight (DW) units using a moisture content of 87 percent in root vegetables (USEPA 1997a; Pennington 1994).

The plant-soil bioconcentration factor for compounds in root vegetables accounts for uptake from soil to the belowground root vegetables or produce. For organics, the following equation, obtained from USEPA (1995c), can be used to calculate values on a soil basis ($\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ soil}}$):

$$Br_{rootveg} = \frac{RCF}{K_{ds}} \tag{28}$$

where K_{ds} (mL/g) describes the partitioning of a compound between soil and pore water.

Air to plant transfer factor for leafy vegetables

The air-to-plant biotransfer factor is defined as the ratio of chemical concentration in aboveground plant parts to the chemical concentration in air.

Calamari et al. (1987) reported a relation for bioconcentration in foliage (plant leaves) as:

$$\log FCF = 1.25 \ \log H + 4.06 \tag{29}$$

where

$$FCF = \frac{\text{concentration in foliage (ng/g DW)}}{\text{concentration in air (ng/g)}}$$

H = Henry's law constant (Pa m^3 mol^{-1})

Equation 29 was developed for chlorinated hydrocarbons in azalea leaves, but PCBs were excluded from the correlation.

USEPA has recommended the equation developed by Bacci et al. (1992) for calculation of the air-to-plant transfer factor (*Bv*) only for aboveground exposed produce (both fruits and vegetables). The aboveground-protected produce (both fruits and vegetables) and belowground produce were assumed to be protected from air-to-plant transfer. According to USEPA (1995c), root vegetables are assumed to be also protected from air-to-plant transfer. Bacci et al. (1992) developed the following equations without distinguishing between forage and aboveground produce,

$$\log B_{vol} = 1.065 \log K_{ow} - \log \left(\frac{H}{RT}\right) - 1.654$$

$$B_v = \frac{\rho_{air} \times B_{vol}}{(1 - f_{water}) \times \rho_{forage}} \quad (30)$$

where

B_{vol} = volumetric air-to-plant biotransfer factor (FW), (μg chemical/L FW plant)(μg chemical/L air)

H = Henry's law constant (atm-m^3/mole)

R = Universal gas constant (atm-m^3/mol-K) = $8.2 \cdot 10^{-5}$ [atm-m^3/mol·K]

T = Temperature 298.1 K [K = 273.16 + °C]

B_v = mass-based air-to-plant biotransfer factor (μg chemical/g DW plant)/(μg chemical/g air)

ρ_{air} = Density of air, 1.19 g/L (Weast 1981)

f_{water} = Fraction of forage that is water, 0.85 (Macrady and Maggard 1993)

ρ_{forage} = Forage density, 770 g/L (Macrady and Maggard 1993)

Note that *FCF* in Equation 29 has the same units as B_v in Equation 30, but the two equations yield different results. Equation 30 was used to calculate transfer factors for the Range Database. It should be noted that uptake of airborne pollutants in vascular plants is a complicated process.

Alternative plant models

In addition to the above equation correlations, other studies have been reported in the literature. Paterson and Mackay (1994) developed a dynamic three-compartment mass balance model of a plant to quantify the uptake of organic chemicals from soil and atmosphere. The three compartments are roots, leaves, and remaining structure, which is mainly stem, but could also include fruits, seed, or tubers. The processes involved are diffusion and bulk flow of a chemical between soil and root, transport within the plant in the phloem, and transpiration streams between root, stem, and exchange between foliage and air and soil and air. The model accounts for metabolism and growth. The model is used widely and has been tested against field data. The model predictions are generally good. Fryer and Collins (2003) evaluated nine plant uptake models against experimental data and found the Paterson and Mackay model to perform probably the most accurate of all for modeling the air uptake. Nevertheless, the model is relatively complex; therefore, Hung and Mackay (1997) simplified it to develop a model containing only readily available parameters. The results of the

simplified version compared well with both the experimental results and the results of Paterson and Mackay (1994). The Paterson and Mackay (1994) model can better simulate actual transport processes and is recommended to research transport processes (Hung and Mackay 1997). The simplified Hung and Mackay (1997) model is more appropriate for risk assessment purposes.

Chrostowski and Foster (1996) developed a methodology for assessing plant uptake of hydrophobic chemicals (such as PCDDs or PCDFs) via air by analyzing the vapor-particulate partitioning behavior of those compounds. This methodology incorporates physicochemical properties and photolytic degradation rates and applies them to assessing environmental concentrations associated with uptake of vapor phase chemicals in plants. Chrostowski and Foster found one major shortcoming of other models that describe air uptake by plants, i.e., that only volatilization is taken into account as an elimination process, and the models do not reflect the photolysis that is likely to occur for PCDDs or PCDFs.

Evaluation of plant models

McLachlan (2000) compared four estimation methods for deriving the plant-air partitioning coefficient. The approaches were the linear method, non-linear method (Trapp and Matthies 1995), two-compartment method (Riederer 1995) and the Müller et al. method (1994). In summary, current methods agree well with each other. The results indicated good agreement among the four methods for predicting the plant-air partitioning coefficient of lindane, anthracene, and 2,2',5,5'-tetrachlorobiphenyl in grass. McLachlan (2000) concluded that much more research is required for an understanding the influence of both the physical-chemical properties and temperature on the plant-air partitioning coefficient.

Fryer and Collins (2003) evaluated nine plant uptake models against experimental data. These models ranged from simple deterministic equilibrium and steady-state risk assessment screening tools to more complex dynamic models that considered physical, chemical, and biological processes in a mechanistic manner. Among the equilibrium and steady-state models, the Trapp and Matthies (1995) model appears to overestimate most significantly the foliage concentration factor in the water uptake scenarios. In the soil uptake scenarios, the Trapp and Matthies (1995) model produced a BCF closer to the experimentally derived values than in the water uptake scenarios. The most probable cause for this difference is the longer exposure duration of the soil-uptake scenario, where equilibrium conditions are more likely established. This could mean that equilibrium and steady-state models should be more accurate for experiments with a longer duration. The predictions of the dynamic, equilibrium, and steady-state models proved to be highly similar for modeling the air uptake, but the dynamic model of Paterson and Mackay (1994) performed probably the most accurately of all. Fryer and Collins (2003) concluded that for the purpose of chronic exposure duration at the screening stage of a risk assessment, the steady-state Trapp and Matthies (1995) model proved to be sufficient. However, it will prove necessary to use a more complex dynamic model if a chemical reaches the plant via the aerial uptake route, because the exposure duration is relatively short in this rapidly changing medium and the source term is not constant.

Other Sources of Data

The ARAMS/FRAMES and RAIS constituent databases were searched for information on the food transfer factors. Table 20 shows available data from ARAMS/FRAMES and Table 21 provides data available from RAIS. Note that the soil-to-plant uptake in Table 21 is the same parameter as soil-to-plant concentration ratio in Table 20. Feed to animal milk transfer in Table 20 has units of days per liter, but in Table 21, it has units of days per kilogram.

Tables 20 and 21 indicate that the available data in both ARAMS/FRAMES and RAIS Databases are limited. The RAIS Database has data for more chemicals than the ARAMS/FRAMES Database, but many of the values in RAIS are default values.

Data Gaps, Conclusions, and Recommendations

Many approaches are available to describe food transfer factors for human exposure. The choice for the most appropriate method depends largely on the scope of the risk assessment. For most purposes, it is often better to use a simple and generic empirical approach than a more demanding mechanistic one. The variation in the different model methods and results can be large.

The two regression equations (Equations 19 and 20) describing the bioconcentration in fish seem sufficiently valid as a compromise between complexity and the accuracy of estimations. Alternative models include the model of Meylan et al. (1999) and Jager and Hamers (1997). Alternative approaches should be evaluated, but they were beyond the scope of this study.

For bioaccumulation into meat and milk, large uncertainties should be expected. There is little room for improvement of the current approach on the basis of the available data sets. It is assumed that the concentration in meat and milk remains constant outside the maximum range of conditions for which the equations were employed, which may be a great overestimation. Further, the steady-state assumption between chemical intake and elimination oversimplifies the behavior or lactating status of a cow. Further research is needed to determine whether the models of Dowdy et al. (1996) or McLachlan (1994) are a better alternative than the Travis and Arms (1988) approach. In view of the importance for hydrophobic chemicals, the route for high log K_{ow} compounds is a main candidate for further investigation. The regressions of Travis and Arms (1988) are based on 25 percent fat for meat and 3.68 percent fat for milk. The fat

Table 20
Food Transfer Factors in ARAMS/FRAMES Constituent Database

ID	Chemical	CAS Number	Parameter											
			A	B	C	D	E	F	G	H	I	J	K	L
1	1,2-dichloroethene (cis)	156-59-2	2.9											
2	1,2-dichloroethene (trans)	156-60-5	2.9											
5	1,2-dichlorethane	107-06-2	2											
9	1,3,5-trinitrobenzene	99-35-4												
10	1,3-butadiene	106-99-0												
11	1,3-dinitrobenzene	99-65-0												
14	1-butanol	71-36-3												
23	2,3,7,8-tetrachlorodibenzo-p-dioxin	1746-01-6			0.055	0.0102								
24	2,4,6-trinitrotoluene (TNT)	118-96-7												
25	2,4-dinitrotoluene (DNT; 2,4-DNT)	121-14-2												
28	2-amino-4,6-dinitrotoluene	35572-78-2												
30	2-butanone	78-93-3												
36	2-nitrotoluene (ONT)	88-72-2												

Parameter Identification

A = Bioaccumulation in freshwater fish (BCF_{fish}) (L/kg)	Data values for 39 chemicals
B = Bioaccumulation in freshwater crustacea (*BCF*) (L/kg)	Data values for 18 chemicals
C = Feed to animal meat transfer factor (days/kg)	Data values for 22 chemicals
D = Feed to animal milk transfer factor (days/L)	Data values for 23 chemicals
E = Soil to plant concentration ratio for leafy vegetables (kg soil /kg dry plant)	Data values for 23 chemicals
F = Soil to plant concentration ratio for root vegetables (kg soil/kg dry plant)	Data values for 21 chemicals
G = Soil to plant concentration ratio for fruit (kg soil/kg dry)	Data values for 21 chemicals
H = Soil to plant concentration ratio for cereal (kg soil/kg dry)	Data values for 21 chemicals
I = Soil to plant concentration ratio for animal forage (kg soil/kg dry)	Data values for 21 chemicals
J = Soil to plant concentration ratio for hay (kg soil/kg dry)	Data values for 21 chemicals
K = Soil to plant concentration ratio for grain (kg soil/kg dry)	Data values for 21 chemicals
L = Soil to plant concentration ratio, other vegetables (kg soil/kg dry)	Data values for 21 chemicals

(Sheet 1 of 5)

Table 20 (Continued)

ID	Chemical	CAS Number	Parameter											
			A	B	C	D	E	F	G	H	I	J	K	L
38	2-propanol	67-63-0												
49	4-methyl-2-pentanone	108-10-1												
52	acenaphthene	83-32-9												
53	acenaphthylene	208-96-8	301											
56	acetone	67-64-1												
57	acetonitrile	75-05-8												
58	acetophenone	98-86-2												
60	acrolein	107-02-8	344											
61	acrylonitrile	107-13-1	48											
62	aluminum	7429-90-5	10	63	0.0015	0.0005	0.00072	0.00072	0.00072	0.00072	0.00072	0.00072	0.00072	0.00072
63	anthracene	120-12-7												
64	antimony	7440-36-0	200	10	0.001	0.0001	0.00013	0.00056	0.00008	0.03	0.00013	0.00013	0.03	0.00056
65	arsenic	7440-38-2	100	40	0.002	0.00006	0.04	0.006	0.006	0.006	0.04	0.04	0.006	0.006
66	barium	7440-39-3	200	0.2	0.00015	0.00035	0.15	0.015	0.015	0.015	0.15	0.15	0.015	0.015
69	benzene	71-43-2												
70	benzo(a)anthracene	56-55-3	11700											
71	benzo(a)pyrene	50-32-8												
72	benzo(b)fluoranthene	205-99-2												
73	benzo(e)pyrene	192-97-2												
75	benzo(k)fluoranthene	207-08-9												
78	beryllium	7440-41-7	19	10	0.0008	0.000002	0.01	0.0015	0.0015	0.0015	0.01	0.01	0.0015	0.0015
79	bis(2-ethylhexyl)phthalate	117-81-7												
81	cadmium	7440-43-9	200	2000	0.00055	0.001	0.55	0.15	0.15	0.15	0.55	0.55	0.15	0.15
82	calcium	7440-70-2					3.5	0.35	0.35	0.35	3.5	3.5	0.35	0.35
84	carbon disulfide	75-15-0												
86	carbontetrachloride	56-23-5	150											
88	chlorobenzene	108-90-7	645											
89	chloroethene (vinyl chloride)	75-01-4												

(Sheet 2 of 5)

Table 20 (Continued)

ID	Chemical	CAS Number	Parameter											
			A	B	C	D	E	F	G	H	I	J	K	L
90	chloroform	67-66-3												
91	chloromethane	74-87-3												
92	chromium	7440-47-3	200	2000	0.0055	0.0015	0.0075	0.0045	0.0045	0.0045	0.0075	0.0075	0.0045	0.0045
93	chrysene	218-01-9												
95	Cl2 (a)	7782-50-5	50		0.08	0.015	70	70	70	70	70	70	70	70
96	cobalt	7440-48-4	50	200	0.001	0.0005	0.081	0.04	0.007	0.0037	0.081	0.081	0.0037	0.04
97	copper	7440-50-8	50	400	0.01	0.0015	0.4	0.25	0.25	0.25	0.4	0.4	0.25	0.25
98	dibenz(a,h)anthracene	53-70-3	113000											
100	dibutyl phthalate	84-74-2												
102	dichlorodiflouromethane	75-71-8												
104	diphenylamine	122-39-4												
105	ethane	74-84-0												
106	ethanol	64-17-5												
107	ethyl benzene	100-41-4												
108	ethyl chloride	75-00-3												
110	fluoranthene	206-44-0												
111	fluorene	86-73-7	713											
112	formaldehyde	50-00-0												
113	furan	110-00-9												
114	HCl	7647-01-0					70	70	70	70	70	70	70	70
116	hexachlorobenzene	118-74-1			0.0447	0.00851								
117	hexachlorobutadiene	87-68-3												
118	hexachlorocyclopentadiene	77-47-4	29											
119	hexachloroethane	67-72-1												
121	hexane	110-54-3												
122	HMX	2691-41-0												
123	hydrogen cyanide	74-90-8												
124	i-butane (isobutane)	75-28-5												

(Sheet 3 of 5)

Table 20 (Continued)

ID	Chemical	CAS Number	Parameter											
			A	B	C	D	E	F	G	H	I	J	K	L
126	indeno(1,2,3-cd)pyrene	193-39-5												
128	lead	7439-92-1	100	100	0.0003	0.00025	0.0058	0.0032	0.009	0.0047	0.0058	0.0058	0.0047	0.0032
129	xylene (mixed isomers)	1330-20-7												
130	m-xylene (meta-xylene)	108-38-3												
131	p-xylene (para-xylene)	106-42-3												
133	manganese	7439-96-5	400	90000	0.0004	0.00035	0.56	0.15	0.05	0.29	0.56	0.56	0.29	0.15
134	m-dichlorobenzene	541-73-1	66											
135	mercury	7439-97-6	1000	200000	0.25	0.00045	0.9	0.2	0.2	0.2	0.9	0.9	0.2	0.2
138	methylene chloride	75-09-2												
142	naphthalene	91-20-3				0.0002								
143	n-butane	106-97-8												
145	NH3 (ammonia)	7664-41-7												
146	nickel	7440-02-0	100	100	0.006	0.001	0.28	0.06	0.06	0.03	0.28	0.28	0.03	0.06
147	nitric acid	7697-37-2	150000		0.075	0.025	7.5	7.5	7.5	7.5	7.5	7.5	7.5	7.5
148	nitrobenzene	98-95-3	15											
152	nonanal	124-19-6												
153	OCDD (1,2,3,4,6,7,8,9-OCDD)	3268-87-9												
155	o-dichlorobenzene	95-50-1	89											
157	o-xylene (ortho-xylene)	95-47-6												
159	p-dichlorobenzene (para-dichlorobenzene)	106-46-7	60											
160	pentaerythritoltetranitrate (PETN)	78-11-5												
161	perchloroethylene	127-18-4	100											
162	phenanthrene	85-01-8												
163	phenol	108-95-2												
165	phosphorus	7723-14-0	70000	20000	0.055	0.015	0.875							

(Sheet 4 of 5)

Table 20 (Concluded)

ID	Chemical	CAS Number	Parameter											
			A	B	C	D	E	F	G	H	I	J	K	L
167	propane	74-98-6												
170	pyrene	129-00-0	2800											
171	RDX	121-82-4												
172	selenium	7782-49-2	170	170	0.015	0.004	0.025	0.025	0.025	0.025	0.025	0.025	0.025	0.025
173	silver	7440-22-4	2.3	770	0.003	0.02	0.00027	0.0013	0.0008	0.1	0.00027	0.00027	0.1	0.0013
174	styrene (vinyl benzene)	100-42-5												
176	sulfuric acid	7664-93-9					1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.5
177	tetryl (2,4,6-trinitrophenylmethylnitramine)	479-45-8												
178	thallium	7440-28-0	10000	15000	0.04	0.002	0.004	0.0004	0.0004	0.0004	0.004	0.004	0.0004	0.0004
180	toluene	108-88-3												
185	trichloroethylene (TCE)	79-01-6	11											
186	trichloroflouromethane	75-69-4												
187	vinylidenechloride	75-35-4												
188	zinc	7440-66-6	2500	10000	0.1	0.01	0.148							
Statistical Analysis														
Number of Available Data			39	18	22	23	23	21	21	21	21	21	21	21
Percent Available Data			21	10	12	12	12	11	11	11	11	11	11	11

(Sheet 5 of 5)

Table 21
Food Transfer Factors in the RAIS Constituent Database

ID	Chemical	CAS Number	A	B	C	D
1	1,2-dichloroethene (cis)	156-59-2	8.1	2.00E-06	6.30E-07	3.00E+00
2	1,2-dichloroethene (trans)	156-60-5	8.1	7.50E-08	2.40E-08	2.00E+01
3	(1,2-dichloroethyl) benzene	1074-11-9				
4	1,2,4-trimethylbenzene	95-63-6	120	1.50E-04	4.80E-05	2.40E-01
5	1,2-dichlorethane	107-06-2	2.8	7.90E-07	2.50E-07	5.10E+00
6	1,2-dichloro-3-methylbenzene	32768-54-0				
7	1,2-dichloroethene (cis/trans mixture)	540-59-0	8.1	7.50E-08	2.40E-08	2.00E+01
8	1,3,5-trimethylbenzene (mesitylene)	108-67-8	86	6.60E-05	2.10E-05	3.90E-01
9	1,3,5-trinitrobenzene	99-35-4	1.6	4.00E-07	1.30E-07	7.70E+00
10	1,3-butadiene	106-99-0	6.8	2.50E-06	7.90E-07	2.60E+00
11	1,3-dinitrobenzene	99-65-0	2.8	1.00E-06	3.10E-07	4.50E+00
12	1,4-diamino-2,3-dihydroanthraquinone (DDA) violet-dye mix	81-63-0				
13	1,4-di-p-toluidinoanthraquinone (PTA) solvent green 3	128-80-3				
14	1-butanol	71-36-3	3.2	1.10E-07	3.50E-08	1.60E+01
15	1-butene	106-98-9				
16	1-chloro-2-methylbenzene	95-49-8	86	6.30E-05	2.00E-05	4.10E-01
17	1-chloro-3-methylbenzene	108-41-8				
18	1-hexene	592-41-6				
19	1-pentene	109-67-1				
20	1-(methylamino)anthraquinone (disperse red 9)	82-38-2				
21	2-(2-quinolyl)-1,3-indandione (D & C yellow no. 11) or (solvent yellow 33)	8003-22-3				
22	2,3-butanedione	625-34-3				
23	2,3,7,8-tetrachlorodibenzo-p-dioxin	1746-01-6	34000	1.60E-01	5.00E-02	4.30E-03
24	2,4,6-trinitrotoluene (TNT)	118-96-7	3.4	5.00E-06	1.60E-06	1.80E+00
25	2,4-dinitrotoluene (DNT; 2,4-DNT)	121-14-2	6.7	2.50E-06	7.90E-07	2.60E+00
26	2,6-dinitrotoluene (2,6-DNT)	606-20-2	8.3	1.30E-06	4.00E-07	3.90E+00
27	2,5-dimethylfuran	625-86-5				
28	2-amino-4,6-dinitrotoluene	35572-78-2	5.2			
29	2-amino-9,10-anthracenedione (a) (AAQ)	117-79-3				
30	2-butanone	78-93-3	3.2	4.70E-08	1.50E-08	2.60E+01
31	2-furaldehyde	98-01-1	3.2	7.90E-05	2.50E-05	3.50E-01
32	2-heptanone	110-43-0				
33	2-methyl-1-butene	563-46-2				
34	2-methylfuran	534-22-5				
35	2-methylthiophene	554-14-3				
36	2-nitrotoluene (ONT)	88-72-2	12	5.00E-06	1.60E-06	1.80E+00
37	2-pentanone	107-87-9				
38	2-propanol	67-63-0	3.2	2.80E-08	8.80E-09	3.60E+01
39	2-thiophenecarboxaldehyde	98-03-3				
40	3-(phenylhydrazone)-1H-indole-2,3-dione					
41	3-furaldehyde	498-60-2				
42	3-methyl-1-butene	563-45-1				

(Sheet 1 of 4)

Note: Some of the values in Table 21 may be default values.

A = Fish bioaccumulation factor, BAF (L/kg)

B = Beef transfer coefficient (days/kg)

C = Milk transfer coefficient (days/kg)

D= Soil-to-plant dry uptake

Table 21 (Continued)

ID	Chemical	CAS Number	A	B	C	D
43	3-methylfuran	930-27-8				
44	3-methylthiophene	616-44-4				
45	3-nitrotoluene	99-08-1	15	6.30E-06	2.00E-06	1.50E+00
46	4-1,2,4-oxadizaolin-3-one-2,5-diphenyl-delta					
47	4-amino-2,6-dinitrotoluene (4ADNT)	19406-51-0				
48	4-ethyltoluene	622-96-8				
49	4-methyl-2-pentanone	108-10-1	2	4.00E-07	1.30E-07	7.70E+00
50	4-nitrotoluene	99-99-0	13	6.30E-06	2.00E-06	1.50E+00
51	4-phenoxy-2(1H)-quinolinone	66662-28-0				
52	acenaphthene	83-32-9	210	5.00E-04	1.60E-04	1.20E-01
53	acenaphthylene	208-96-8	220	1.30E-04	4.00E-05	2.70E-01
54	acetaldehyde	75-07-0	3.2	1.50E-08	4.80E-09	5.10E+01
55	acetic acid	64-19-7				
56	acetone	67-64-1	3.2	1.40E-08	4.50E-09	5.20E+01
57	acetonitrile	75-05-8	3.2	1.10E-08	3.60E-09	6.00E+01
58	acetophenone	98-86-2	0.47	1.30E-06	4.00E-07	3.90E+00
59	acetylene	74-86-2				
60	acrolein	107-02-8	3.2	2.00E-08	6.30E-09	4.30E+01
61	acrylonitrile	107-13-1	3.2	4.40E-08	1.40E-08	2.70E+01
62	aluminum	7429-90-5	3.2	1.50E-03	2.00E-04	4.00E-03
63	anthracene	120-12-7	530	6.30E-04	2.00E-04	1.10E-01
64	antimony	7440-36-0	3.2	4.00E-05	2.50E-05	5.00E-02
65	arsenic	7440-38-2	3.2	2.00E-03	6.00E-05	4.00E-02
66	barium	7440-39-3	3.2	2.00E-04	4.80E-04	1.00E-01
67	benzaldehyde	100-52-7	2.8	5.00E-06	1.60E-06	1.80E+00
68	benzanthrone (b)	82-05-3				
69	benzene	71-43-2	8.7	3.10E-06	9.90E-07	2.30E+00
70	benzo(a)anthracene	56-55-3	5400	1.30E-02	4.00E-03	1.90E-02
71	benzo(a)pyrene	50-32-8	11000	3.10E-02	9.90E-03	1.10E-02
72	benzo(b)fluoranthene	205-99-2	5600	3.10E-02	9.90E-03	1.10E-02
73	benzo(e)pyrene	192-97-2				
74	benzo(g,h,i)perylene	191-24-2	25000	1.00E-01	3.10E-02	5.60E-03
75	benzo(k)fluoranthene	207-08-9	10000	1.60E-01	5.00E-02	4.30E-03
76	benzofuran	271-89-6				
77	benzonitrile	100-47-0				
78	beryllium	7440-41-7	3.2	1.00E-03	9.00E-07	1.00E-02
79	bis(2-ethylhexyl)phthalate	117-81-7	310	2.00E-03	6.30E-04	5.50E-02
80	butanal	123-72-8				
81	cadmium	7440-43-9	3.2	4.00E-04	1.00E-03	5.50E-01
82	calcium	7440-70-2				
83	carbon dioxide (CO2)	124-38-9				
84	carbon disulfide	75-15-0	6.2	4.00E-06	1.30E-06	2.00E+00
85	carbon monoxide (CO)	630-08-0				
86	carbon tetrachloride	56-23-5	30	1.60E-05	5.00E-06	9.00E-01
87	carbonyl sulfide	463-58-1				
88	chlorobenzene	108-90-7	31	1.60E-05	5.00E-06	9.00E-01
89	chloroethene (vinyl chloride)	75-01-4	3.5	6.30E-07	2.00E-07	5.90E+00
90	chloroform	67-66-3	6.6	2.50E-06	7.90E-07	2.60E+00
91	chloromethane	74-87-3	3.2	2.00E-07	6.40E-08	1.10E+01
92	chromium	7440-47-3				
93	chrysene	218-01-9	5900	1.30E-02	4.00E-03	1.90E-02

(Sheet 2 of 4)

Table 21 (Continued)

ID	Chemical	CAS Number	A	B	C	D
94	cis-2-butene	590-18-1				
95	Cl2 (a)	7782-50-5	3.2	2.00E-02	1.70E-02	7.00E+01
96	cobalt	7440-48-4	3.2	1.00E-04	7.00E-05	5.40E-02
97	copper	7440-50-8	3.2	9.00E-03	1.50E-03	8.00E-01
98	dibenz(a,h)anthracene	53-70-3	22000	1.60E-01	5.00E-02	4.30E-03
99	dibenzo(b,def)chrysene-7,14 dione (c.i. vat yellow 4)	128-66-5				
100	dibutyl phthalate	84-74-2	580	2.00E-03	6.30E-04	5.50E-02
101	dichloroacetonitrile	3018-12-0				
102	dichlorodiflouromethane	75-71-8	9.2	4.00E-06	1.30E-06	2.00E+00
103	dimethyltrisulfide	3658-80-8				
104	diphenylamine	122-39-4	99	7.90E-05	2.50E-05	3.50E-01
105	ethane	74-84-0				
106	ethanol	64-17-5				
107	ethyl benzene	100-41-4	53	3.10E-05	9.90E-06	6.10E-01
108	ethyl chloride	75-00-3	2.5	6.30E-07	2.00E-07	5.90E+00
109	ethylene	74-85-1				
110	fluoranthene	206-44-0	1900	2.00E-03	6.30E-04	5.50E-02
111	fluorene	86-73-7	330	6.30E-04	2.00E-04	1.10E-01
112	formaldehyde	50-00-0	3.2	2.50E-08	7.90E-09	3.80E+01
113	furan	110-00-9	2.1	5.00E-07	1.60E-07	6.70E+00
114	HCl	7647-01-0	3.2			
115	heptanal	111-71-7				
116	hexachlorobenzene	118-74-1	5200	5.00E-03	1.60E-03	3.20E-02
117	hexachlorobutadiene	87-68-3	960	1.60E-03	5.00E-04	6.20E-02
118	hexachlorocyclopentadiene	77-47-4	1500	2.50E-04	7.90E-05	1.80E-01
119	hexachloroethane	67-72-1	310	2.00E-04	6.30E-05	2.10E-01
120	hexanal	66-25-1				
121	hexane	110-54-3	200	2.00E-04	6.30E-05	2.10E-01
122	HMX	2691-41-0	3.2	9.70E-08	3.10E-08	1.70E+01
123	hydrogen cyanide	74-90-8	3.2	6.00E-08	1.90E-08	2.30E+01
124	i-butane (isobutane)	75-28-5				
125	i-butene (isobutene/e-butylene)	115-11-7				
126	indeno(1,2,3-cd)pyrene	193-39-5	29000	1.00E-01	3.10E-02	5.60E-03
127	isothiocyanatomethane	556-61-6				
128	lead	7439-92-1	3.2	4.00E-04	3.00E-04	9.00E-02
129	xylene (mixed isomers)	1330-20-7	50	5.00E-05	1.60E-05	4.60E-01
130	m-xylene (meta-xylene)	108-38-3	58	4.00E-05	1.30E-05	5.30E-01
131	p-xylene (para-xylene)	106-42-3	53	4.00E-05	1.30E-05	5.30E-01
132	magnesium	7439-95-4	3.2	5.00E-03	4.00E-03	1.00E+00
133	manganese	7439-96-5	3.2	5.00E-04	3.00E-05	6.80E-01
134	m-dichlorobenzene	541-73-1	100	1.00E-04	3.10E-05	3.10E-01
135	mercury	7439-97-6	3.2	1.00E-02	4.70E-04	1.00E+00
136	methacrolein	78-85-3				
137	methane	74-82-8				
138	methylene chloride	75-09-2	1.8	5.00E-07	1.60E-07	6.70E+00
139	methylnitrite	624-91-9				
140	methyl-t-butylether (MTBE)	1634-04-4	3.2	2.20E-07	6.90E-08	1.10E+01
141	methyl-vinyl ketone	78-94-4				
142	naphthalene	91-20-3	69	5.00E-05	1.60E-05	4.60E-01
143	n-butane	106-97-8				
144	n-decane	124-18-5				

(Sheet 3 of 4)

Table 21 (Concluded)

ID	Chemical	CAS Number	A	B	C	D
145	NH3 (ammonia)	7664-41-7	3.2	2.50E-08	7.90E-09	3.80E+01
146	nickel	7440-02-0	3.2	5.00E-03	1.60E-02	1.80E-01
147	nitric acid	7697-37-2				
148	nitrobenzene	98-95-3	5.3	1.60E-06	5.00E-07	3.40E+00
149	nitrogen oxide (NOx)	10102-44-0	3.2			
150	nitroglycerine	55-63-0				
151	nitromethane	75-52-5				
152	nonanal	124-19-6				
153	OCDD (1,2,3,4,6,7,8,9-OCDD)	3268-87-9	24	1.50E+01	4.80E+00	3.10E-04
154	octanal	124-13-0				
155	o-dichlorobenzene	95-50-1	87	6.30E-05	2.00E-05	4.10E-01
156	o-methoxy-phenyl-azo-b-naphthol (oil red g)	1229-55-6				
157	o-xylene (ortho-xylene)	95-47-6	50	4.00E-05	1.30E-05	5.30E-01
158	particulate cyanide	57-12-5				
159	p-dichlorobenzene (para-dichlorobenzene)	106-46-7	89	6.30E-05	2.00E-05	4.10E-01
160	pentaerythritoltetranitrate (PETN)	78-11-5				
161	perchloroethylene	127-18-4	83	1.00E-05	3.10E-06	1.20E+00
162	phenanthrene	85-01-8	540	1.00E-03	3.10E-04	8.20E-02
163	phenol	108-95-2	2.7	7.90E-07	2.50E-07	5.10E+00
164	phenylacetylene (ethynyl benzene)	536-74-3				
165	phosphorus	7723-14-0	3.2			
166	propanal	123-38-6				
167	propane	74-98-6				
168	propylene	115-07-1				
169	propyne	74-99-7				
170	pyrene	129-00-0	1100	2.00E-03	6.30E-04	5.50E-02
171	RDX	121-82-4	3.2	5.00E-05	1.60E-05	4.60E-01
172	selenium	7782-49-2	3.2	1.00E-01	1.00E-02	5.00E-01
173	silver	7440-22-4	3.2	3.00E-03	5.00E-05	1.00E+00
174	styrene (vinyl benzene)	100-42-5	37	2.00E-05	6.30E-06	7.90E-01
175	sulfur dioxide (SO2)	7446-09-5				
176	sulfuric acid	7664-93-9				
177	tetryl (2,4,6-trinitrophenylmethylnitramine)	479-45-8	3.7	2.50E-06	7.90E-07	2.60E+00
178	thallium	7440-28-0	3.2	4.00E-02	2.00E-03	4.00E-03
179	thiophene	110-02-1				
180	toluene	108-88-3	25	1.30E-05	4.00E-06	1.00E+00
181	trans-2-butenal	123-73-9	3.2	1.60E-06	5.00E-07	3.40E+00
182	trans-2-butene	624-64-6				
183	trans-2-pentene	646-04-8				
184	trans-3-penten-2-one	625-33-2				
185	trichloroethylene (TCE)	79-01-6	15	6.30E-06	2.00E-06	1.50E+00
186	trichloroflouromethane	75-69-4	18	7.90E-06	2.50E-06	1.30E+00
187	vinylidenechloride	75-35-4	8.7	1.60E-06	5.00E-07	3.40E+00
188	zinc	7440-66-6	3.2	1.00E-01	1.00E-02	9.90E-01
Number of available data			111	107	107	107
Percent available data			59	57	57	57

(Sheet 4 of 4)

content used for meat is rather high. All milk products are represented by milk, which is not valid for the much fattier milk products such as cheese and butter. Perhaps it is better to relate concentrations in meat and milk to fat content. Also, cattle were not exposed to other fodder types, other than grass. Due to this

assumption, the model calculations represent a conservative situation since the concentration in other fodder may be significantly lower than in grass. The degree of conservatism is unknown.

The Range Database will include data from the ARAMS/FRAMES (Table 20) and RAIS (Table 21) Databases. Equation 19 for fish bioconcentration factor, Equation 21 for biotransfer factor for beef, Equation 22 for biotransfer factor for milk, Equation 23 for biotransfer factor for pork, Equation 24 for biotransfer factor for chicken, and Equation 25 for biotransfer factor for poultry eggs will be used to generate food transfer factors for organic chemicals in the Range Database. For inorganic constituents, values recommended by USEPA and data from Figures 2-5 will be added to the database.

The steady-state model of Travis and Arms (1988) is appropriate for the soil-to-crop uptake routes (Equation 26). The empirical plant model by Briggs et al. (1982) (Equation 27) and Equation 28 can be used to compute root plant-soil bioconcentration factors. The model by Bacci et al. (1992), Equation 30, is recommended for air to plant uptake.

Experimentally measured food transfer factors are not available for many of the chemicals in the Range Database. Several empirical mathematical correlations have been developed that provide approximate values that should be suitable for most studies. There are very large data gaps for saltwater fish. The empirical models for fish may be modified for a marine environment, but data are required for this. Thus, existing models must be used with care for marine fish. The bulk of the consumed fish is retrieved from the marine water environment and not from the freshwater environment. Thus, food transfer factors for marine food should receive future attention.

Table 22
Recommended Equations and Other Data for Human Food Transfer Factors (Aquatic, Animal, and Plant)

Property	Unit	Source		
		Equation Number (Organics)	Table	Figure (Inorganics)
Bioaccumulation in freshwater fish	L/kg	19	18, 20, 21, 39	
Bioaccumulation in freshwater mollusk	L/kg			
Bioaccumulation in freshwater crustacea	L/kg		20	
Bioaccumulation in freshwater plants	L/kg			
Bioaccumulation in saltwater fish	L/kg			
Bioaccumulation in saltwater mollusk	L/kg			
Bioaccumulation in saltwater crustacea	L/kg			
Bioaccumulation in saltwater plants	L/kg			
Feed to beef transfer factor	days/kg	21	20, 21	2
Feed to milk transfer factor	days/L	22	20, 21[1]	3
Feed to pork transfer factor	days/kg	23		
Feed to poultry transfer factor	days/kg	24		
Feed to egg transfer factor	days/kg	25		
Soil to plant concentration ratio for leafy vegetables	kg soil/kg dry)	26	20, 21[2]	4
Soil to plant concentration ratio for root vegetables	kg soil/kg (dry)	27 & 28	20	
Soil to plant concentration ratio for fruit	kg soil/kg (dry)	26	20	5
Soil to plant concentration ratio for cereal	kg soil/kg (dry)	26	20	
Soil to plant concentration ratio for animal forage	kg soil/kg (dry)	26	20, 21[2]	
Soil to plant concentration ratio for hay	kg soil/kg (dry)	26	20, 21[2]	
Soil to plant concentration ratio for grain	kg soil/kg (dry)	26	20	
Soil to plant concentration ratio, other vegetables	kg soil/kg (dry)	26	20	
Root concentration factor	mg/kg per mg/kg	27		
Air to plant transfer factor for leafy vegetables	mg/kg per mg/kg	30		
Air to plant transfer factor for forage	mg/kg per mg/kg			

[1] In RAIS Database milk transfer coefficient has different units than in ARAMS/FRAMES Database.

[2] In RAIS Database this parameter is identified as soil-to-plant-dry uptake.

6 Environmental Degradation Rates and Half-Lives

Introduction

There have been many publications of degradation rates of chemical compounds in the environment. However, even for well-studied compounds there is often disagreement in publications as to the values of the degradation rates, even under similar environmental conditions. This problem is familiar for other properties and parameters but is most exacerbated for environmental degradation rates, in part because of the complex mixture usually characteristic of environmental matrices and in part because of natural variation between similar matrices in different locations. Varying environmental conditions among locations also play an important role.

This study undertook to find published measured values and/or software to predict values for the properties and parameters for the 188 constituents considered in this project for development of the Range Database. A number of environmental matrices, situations, and process were considered. Biodegradation when present is most often the most dominant degradation process.

Environmental degradation rates or half-lives that were considered in this study included:

a. Half-life in air (process not specified).

b. Half-life in groundwater (process not specified).

c. Half-life in surface water (process not specified).

d. Half-life in soil (process not specified).

e. Oxidation half-life in air.

f. Hydrolysis half-life in water.

g. Photodegradation half-life in air.

h. Photodegradation half-life in water.

i. Biodegradation half-life in air.

j. Biodegradation half-life in water.

k. Biodegradation half-life in soil.

Methods

There are many journals that publish articles containing degradation rates of some of these compounds. Perhaps the most generally prominent is *Environmental Science & Technology*, whereas others such as *Biodegradation* and *SAR and QSAR in Environmental Research* are more specialized. There are very few compendiums containing many degradation rates together. One is the *Physical-Chemical Properties and Environmental Fate and Degradation Handbook* by Mackay et al. (2000). These and others are listed in the References.

Many of the compounds considered in this study have military significance and have been studied by researchers in Army and other DoD laboratories. For environmental consequences, ERDC has been the source of the most publications, with contributions also from AEC and CHPPM. Most of the values for these compounds found in publications were compiled into the ARAMS Range Database (http://el.erdc.usace.army.mil/arams/) as reported in Zakikhani et al. (2002). The classification scheme of Mackay et al. (2000) was broadly followed.

There are many data gaps, however, particularly for degradation rates. Therefore, QSAR software packages that could be predictive of environmental degradations rates needed to fill the gaps were examined. Most QSAR software concentrates on equilibrium mass balance and partitioning behavior such as K_{ow}, with very little reactivity considerations. Some QSAR packages attempt to be predictive of toxicity, at least under specified conditions. Furthermore, for the most part, all of these are only for special classes of compounds, not encompassing the broad range of Range Database compounds.

Database Enumeration

The USEPA has a number of databases and software packages relating to environmental QSAR. For the most part these packages, such as ASTER, ECOSAR, AMSOL, and CSMoS, are indeed almost entirely partitioning, mass balance, and toxicity. Only two generate estimates of environmental degradation rates and half-lives. These two are the Estimation Programs Interface (EPI) Suite and the Persistence Bioaccumulation Toxicity (PBT) Profiler. EPI and PBT have Windows® versions available, and for this study EPI version 3.12 (http://www.epa.gov/oppt/exposure/docs/episuitedl.htm) was run as well as PBT P2 version 6.00 (http://www.epa.gov/oppt/p2framework/).

Input to these packages was prepared from the ARAMS Range Database, and these were run in batch mode for the 188 Range Database chemicals. These packages take a known or unknown compound in SMILES (Simplified Molecular Input Line Entry Specification) format (http://www.daylight.com/dayhtml/smiles/).

EPI provided results for all compounds, whereas PBT does not output certain data--for instance, metallic elements and some compounds lack effective organic functional groups as described below. For those chemicals for which PBT caveats yield no results, the EPI results are suspect also, for the same reasons given in the PBT documentation.

For both EPI and PBT, the functional group concept is most important. The behavior of a molecule is considered to be the sum of its relevant parts, defined as its functional groups. In fact, EPI and PBT are merely slightly different implementations of the same assumptions and equations.

In both, half-lives for air, water, soil, and sediment are output. Aerobic conditions are assumed, and there is a functional group fit from a linear or nonlinear fit as explained in the BIOWIN documentation (Boethling et al. 1994). Sediment is briefly considered to be anaerobic soil, with overall conversion factors, and water is aerobic (surface) water. Groundwater is not performed explicitly by these packages.

Some of the pertinent documentation is reproduced below in explanation of the calculation methods. Air degradation is considered to be a molecular-mechanical process. The PBT profiler calculates an atmospheric half-life by determining the importance of a chemical's reaction with two of the most prevalent atmospheric oxidants, hydroxyl radicals and ozone. The half-life is calculated directly from gas-phase hydroxyl radical and ozone reaction rate constants. These rate constants are obtained from a database of measured values or, if no experimental values are available, they are estimated using the method of Atkinson (Meylan and Howard 1993). The half-life is calculated from the rate constant and an average atmospheric concentration of these oxidants based on a 24-hr day (Prinn et al. 1992; Atkinson and Carter 1984).

The atmospheric half-life for each process (the chemical's reaction with prevalent atmospheric oxidants) is calculated as follows:

Hydroxyl radicals:

$$t_{1/2} = 0.693/(\text{rate constant cm}^3\text{/molecule-sec} \times 5 \times 10^5 \text{ molecules/cm}^3 \times 86400 \text{ sec/day})$$

Ozone:

$$t_{1/2} = 0.693/(\text{rate constant cm}^3\text{/molecule-sec} \times 7 \times 10^{11} \text{ molecules/cm}^3 \times 86400 \text{ sec/day})$$

and the overall half-life is obtained as:

$$1/t_{1/2}\text{overall} = 1/t_{1/2}\ \text{Hydroxyl radicals} + 1/t_{1/2}\ \text{Ozone}$$

Degradation in other environmental matrices such as water and soil is dominated by microbial biodegradation when it occurs, principally aerobic degradation unless otherwise specified. "The half-life for degradation of a chemical in water, soil, and sediment is determined using the ultimate biodegradation expert survey module of the BIOWIN estimation program" (Boethling et al. 1994). This estimation program provides an indication of a chemical's environmental biodegradation rate in relative terms such as hours, hours to days, days, days to weeks, and so on; the terms represent the approximate amount of time needed for degradation to be "complete." This output cannot be directly compared to established half-life criteria for purposes of identifying chemicals with PBT characteristics, nor can it be used directly by the level III multimedia mass balance model. The mean value within the estimated time range returned by the ultimate biodegradation survey model is converted to a half-life using a set of conversion factors. These conversion factors consider that six half-lives constitute "complete" degradation of a chemical substance (assuming first-order kinetics).

EPI also does some process-specific calculations. For each environmental matrix, however, the degradation processes in EPI and PBT do not explicitly include losses by transport such as volatilization. What the software calls oxidation in air is essentially photolysis (12-hr daylight days) plus oxidation, the quasi-steady photoproduction of ozone and hydroxide, subsequently reacting on low vapor concentrations of compounds of interest. This combination process is supposed to be the most relevant combination for atmospheric degradation of vapors. Very few compounds had calculable water hydrolysis values output, a major shortcoming of this version of the EPI software. Photodegradation is not output explicitly. Photolysis is, therefore, only part of air, and not significant for soil. Significant biodegradation of the vapor in air phase does not really occur.

Analysis

The EPI biodegradation rate in aerobic water is the basis for the other biodegradation rates, with simple overall numerical ratios (not compound specific). For EPI, the half-life in soil is the same as in water, whereas sediment is four times slower. For PBT, soil lives are twice that of water and sediment is nine times that of water. In these expert-system approaches, there is no continuum but discrete half-life ranges of short, medium, and long, typified for the class of explosives--e.g. nitromethane, PETN, and TNT. However, the ranges have a short time spread. Short is 2 weeks, medium is 1 month, long is 2 months. The air half-lives for PBT are almost 1.5 times that for EPI, despite being based on the same information.

All the degradation processes are considered to be first-order in the parent compound, which will be the case for low concentrations and other situations in

which nonlinearities due to rate-limiting steps are not important. In first-order degradation, the concentration decays as follows:

$$c(t) = c(0) \times \exp(-a \times t) \tag{31}$$

where a is the kinetic parameter or decay rate constant. The half-life is then

$$t_{1/2} = \frac{\ln(2)}{a} \tag{32}$$

All the degradation rates were converted to terms of half-lives reported as days for inter-comparison.

Results

The EPI and PBT environmental matrices results are presented in Table 23, whereas the EPI process-specific results are presented in Table 24. These data are compared with each other and with the Range Database data previously compiled from the literature. Table 25 gives the average bias and percent AME. The models all have large negative bias, especially for degradation rates in soil, and extremely large AMEs.

Many compounds have multiple entries for some degradation rates in the previously compiled values in the Range Database. These are not all from the same references, but it is convenient for graphical purposes to group all first entry (including sole entry) values as "database 1," all second entries if any as "database 2," and all third entries as "database 3." There were no degradation parameters in this database with more than three entries per compound. For each degradation parameter, each model prediction was compared to each corresponding database entry, then averaged over entries for each compound and then averaged over the compounds. Thus, each database entry was compared with up to two model predictions, whereas each model prediction was compared with up to three database entries.

Figures 6 and 7 illustrate the comparison between the previous Range Database values and the predicted values for the half-lives in air, in log-log plots, for PBT and EPI, respectively. The Range Database values that agree better with predicted values tend to be also themselves predicted values. Many of the air half-lives already in the database were predicted values. Even for these air degradation rates that provided the most visually pleasing fits, the AMEs were thousands of percent, whereas the negative biases were hundreds of days. It should be noted that the number of comparisons included over 100 compounds over a broad range of compounds.

The model soil degradation rates and water degradation rates correlated very poorly with the database values. The soil AMEs were thousands of percent, and the negative biases were as large as a million days. These huge biases were the

Table 23
EPI and PBT Environmental Matrices Results

Chemical	CAS Number	Half-Life, days							
		Air		Water		Soil		Sediment	
		EPI	PBT	EPI	PBT	EPI	PBT	EPI	PBT
1,2-dichloroethene (cis)	156-59-2	4.11E+00	5.8	3.75E+01	38	3.75E+01	75	1.50E+02	340
1,2-dichloroethene (trans)	156-60-5	4.11E+00	5.8	3.75E+01	38	3.75E+01	75	1.50E+02	340
(1,2-dichloroethyl) benzene	1074-11-9	4.45E+00	6.7	3.75E+01	38	3.75E+01	75	1.50E+02	340
1,2,4-trimethylbenzene	95-63-6	3.29E-01	0.5	3.75E+01	38	3.75E+01	75	1.50E+02	340
1,2-dichlorethane	107-06-2	4.31E+01	67	3.75E+01	38	3.75E+01	75	1.50E+02	340
1,2-dichloro-3-methylbenzene	32768-54-0	9.05E+00	14	3.75E+01	38	3.75E+01	75	1.50E+02	340
1,2-dichloroethene (cis/trans mixture)	540-59-0	4.11E+00	5.8	3.75E+01	38	3.75E+01	75	1.50E+02	340
1,3,5-trimethylbenzene (mesitylene)	108-67-8	1.86E-01	0.28	3.75E+01	38	3.75E+01	75	1.50E+02	340
1,3,5-trinitrobenzene	99-35-4	8.23E+03	12	6.00E+01	60	6.00E+01	120	2.40E+02	540
1,3-butadiene	106-99-0	1.44E-01	0.2	1.50E+01	15	1.50E+01	30	6.00E+01	140
1,3-dinitrobenzene	99-65-0	3.51E+02	540	3.75E+01	38	3.75E+01	75	1.50E+02	340
1,4-diamino-2,3-dihydroanthraquinone (DDA) violet-dye mix	81-63-0	6.20E-02	0.07	3.75E+01	38	3.75E+01	75	1.50E+02	340
1,4-di-p-toluidinoanthraquinone (PTA) solvent green 3	128-80-3	5.34E-02	0.07	6.00E+01	60	6.00E+01	120	2.40E+02	540
1-butanol	71-36-3	1.25E+00	1.9	8.67E+00	8.7	8.67E+00	17	3.47E+01	78
1-butene	106-98-9	2.57E-01	0.34	8.67E+00	8.7	8.67E+00	17	3.47E+01	78
1-chloro-2-methylbenzene	95-49-8	5.88E+00	8.8	3.75E+01	38	3.75E+01	75	1.50E+02	340
1-chloro-3-methylbenzene	108-41-8	2.88E+00	4.2	3.75E+01	38	3.75E+01	75	1.50E+02	340
1-hexene	592-41-6	2.21E-01	0.3	8.67E+00	8.7	8.67E+00	17	3.47E+01	78
1-pentene	109-67-1	2.59E-01	0.35	8.67E+00	8.7	8.67E+00	17	3.47E+01	78
1-(methylamino)anthraquinone (disperse red 9)	82-38-2	5.81E-01	0.88	3.75E+01	38	3.75E+01	75	1.50E+02	340
2-(2-quinolyl)-1,3-indandione (D & C yellow no. 11) or (solvent yellow 33)	8003-22-3	3.69E-01	0.54	3.75E+01	38	3.75E+01	75	1.50E+02	340
2,3-butanedione	431-03-8	4.50E+01	67	1.50E+01	15	1.50E+01	30	6.00E+01	140

(Sheet 1 of 8)

Table 23 (Continued)

Chemical	CAS Number	Half-Life, days							
		Air		Water		Soil		Sediment	
		EPI	PBT	EPI	PBT	EPI	PBT	EPI	PBT
2,3,7,8-tetrachlorodibenzo-p-dioxin	1746-01-6	1.42E+01	21	1.50E+02	180	1.50E+02	360	6.00E+02	1600
2,4,6-trinitrotoluene (TNT)	118-96-7	7.78E+01	120	6.00E+01	60	6.00E+01	120	2.40E+02	540
2,4-dinitrotoluene (DNT; 2,4-DNT)	121-14-2	4.96E+01	75	3.75E+01	38	3.75E+01	75	1.50E+02	340
2,6-dinitrotoluene (2,6-DNT)	606-20-2	4.96E+01	75	3.75E+01	38	3.75E+01	75	1.50E+02	340
2,5-dimethylfuran	625-86-5	8.10E-02	0.12	1.50E+01	15	1.50E+01	30	6.00E+01	140
2-amino-4,6-dinitrotoluene	35572-78-2	9.35E+00	14	6.00E+01	60	6.00E+01	120	2.40E+02	540
2-amino-9,10-anthracenedione (a) (AAQ)	117-79-3	2.54E-01	0.38	3.75E+01	38	3.75E+01	75	1.50E+02	340
2-butanone	78-93-3	9.30E+00	14	1.50E+01	15	1.50E+01	30	6.00E+01	140
2-furaldehyde	98-01-1	3.05E-01	0.46	1.50E+01	15	1.50E+01	30	6.00E+01	140
2-heptanone	110-43-0	9.14E-01	1.4	1.50E+01	15	1.50E+01	30	6.00E+01	140
2-methyl-1-butene	563-46-2	1.48E-01	0.2	1.50E+01	15	1.50E+01	30	6.00E+01	140
2-methylfuran	534-22-5	1.73E-01	0.26	1.50E+01	15	1.50E+01	30	6.00E+01	140
2-methylthiophene	554-14-3	4.28E-01	0.62	1.50E+01	15	1.50E+01	30	6.00E+01	140
2-nitrotoluene (ONT)	88-72-2	1.53E+01	23	3.75E+01	38	3.75E+01	75	1.50E+02	340
2-pentanone	107-87-9	2.30E+00	3.5	1.50E+01	15	1.50E+01	30	6.00E+01	140
2-propanol	67-63-0	2.11E+00	3.2	1.50E+01	15	1.50E+01	30	6.00E+01	140
2-thiophenecarboxaldehyde	98-03-3	4.93E-01	0.75	1.50E+01	15	1.50E+01	30	6.00E+01	140
3-(phenylhydrazone)-1H-indole-2,3-dione	17310-26-8	1.86E-01	0.28	3.75E+01	38	3.75E+01	75	1.50E+02	340
3-furaldehyde	498-60-2	2.21E-01	0.33	1.50E+01	15	1.50E+01	30	6.00E+01	140
3-methyl-1-butene	563-45-1	2.63E-01	0.35	1.50E+01	15	1.50E+01	30	6.00E+01	140
3-methylfuran	930-27-8	1.14E-01	0.17	1.50E+01	15	1.50E+01	30	6.00E+01	140
3-methylthiophene	616-44-4	4.28E-01	0.62	1.50E+01	15	1.50E+01	30	6.00E+01	140
3-nitrotoluene	99-08-1	1.13E+01	17	3.75E+01	38	3.75E+01	75	1.50E+02	340

Table 23 (Continued)

Chemical	CAS Number	Half-Life, days							
		Air		Water		Soil		Sediment	
		EPI	PBT	EPI	PBT	EPI	PBT	EPI	PBT
4-1,2,4-oxadizaolin-3-one-2,5-diphenyl-delta		6.40E-01	0.96	3.75E+01	38	3.75E+01	75	1.50E+02	340
4-amino-2,6-dinitrotoluene (4ADNT)	19406-51-0	9.35E+00	14	6.00E+01	60	6.00E+01	120	2.40E+02	540
4-ethyltoluene	622-96-8	8.84E-01	1.3	1.50E+01	15	1.50E+01	30	6.00E+01	140
4-methyl-2-pentanone	108-10-1	7.59E-01	1.1	1.50E+01	15	1.50E+01	30	6.00E+01	140
4-nitrotoluene	99-99-0	1.39E+01	21	3.75E+01	38	3.75E+01	75	1.50E+02	340
4-phenoxy-2(1H)-quinolinone	66662-28-0	5.63E-02	0.06	3.75E+01	38	3.75E+01	75	1.50E+02	340
acenaphthene	83-32-9	1.84E-01	0.27	3.75E+01	38	3.75E+01	75	1.50E+02	340
acenaphthylene	208-96-8	3.10E-02	0.03	1.50E+01	15	1.50E+01	30	6.00E+01	140
acetaldehyde	75-07-0	6.77E-01	1	1.50E+01	15	1.50E+01	30	6.00E+01	140
acetic acid	64-19-7	1.45E+01	22	8.67E+00	8.7	8.67E+00	17	3.47E+01	78
acetone	67-64-1	4.88E+01	75	1.50E+01	15	1.50E+01	30	6.00E+01	140
acetonitrile	75-05-8	6.43E+01	67	1.50E+01	15	1.50E+01	30	6.00E+01	140
acetophenone	98-86-2	3.90E+00	5.8	1.50E+01	15	1.50E+01	30	6.00E+01	140
acetylene	74-86-2	1.24E+01	18	1.50E+01	15	1.50E+01	30	6.00E+01	140
acrolein	107-02-8	5.30E-01	0.79	1.50E+01	15	1.50E+01	30	6.00E+01	140
acrylonitrile	107-13-1	2.56E+00	3.8	1.50E+01	15	1.50E+01	30	6.00E+01	140
aluminum	7429-90-5	4.17E+03		1.50E+01		1.50E+01		6.00E+01	
anthracene	120-12-7	2.67E-01	0.4	6.00E+01	60	6.00E+01	120	2.40E+02	540
antimony	7440-36-0	4.17E+03		1.50E+01		1.50E+01		6.00E+01	
arsenic	7440-38-2	4.17E+03		1.50E+01		1.50E+01		6.00E+01	
barium	7440-39-3	4.17E+03		1.50E+01		1.50E+01		6.00E+01	
benzaldehyde	100-52-7	8.29E-01	1.2	1.50E+01	15	1.50E+01	30	6.00E+01	140
benzanthrone (b)	82-05-3	5.94E-01	0.88	3.75E+01	38	3.75E+01	75	1.50E+02	340
benzene	71-43-2	8.70E+00	13	3.75E+01	38	3.75E+01	75	1.50E+02	340

Table 23 (Continued)

Chemical	CAS Number	Half-Life, days							
		Air		Water		Soil		Sediment	
		EPI	PBT	EPI	PBT	EPI	PBT	EPI	PBT
benzo(a)anthracene	56-55-3	2.14E-01	0.32	6.00E+01	60	6.00E+01	120	2.40E+02	540
benzo(a)pyrene	50-32-8	2.14E-01	0.32	6.00E+01	60	6.00E+01	120	2.40E+02	540
benzo(b)fluoranthene	205-99-2	5.77E-01	0.88	6.00E+01	60	6.00E+01	120	2.40E+02	540
benzo(e)pyrene	192-97-2	2.14E-01	0.32	6.00E+01	60	6.00E+01	120	2.40E+02	540
benzo(g,h,i)perylene	191-24-2	1.23E-01	0.18	6.00E+01	60	6.00E+01	120	2.40E+02	540
benzo(k)fluoranthene	207-08-9	2.00E-01	0.3	6.00E+01	60	6.00E+01	120	2.40E+02	540
benzofuran	271-89-6	2.87E-01	0.42	1.50E+01	15	1.50E+01	30	6.00E+01	140
benzonitrile	100-47-0	3.24E+01	50	1.50E+01	15	1.50E+01	30	6.00E+01	140
beryllium	7440-41-7	4.17E+03		1.50E+01		1.50E+01		6.00E+01	
bis(2-ethylhexyl)phthalate	117-81-7	4.87E-01	0.75	1.50E+01	15	1.50E+01	30	6.00E+01	140
butanal	123-72-8	4.55E-01	0.67	1.50E+01	15	1.50E+01	30	6.00E+01	140
cadmium	7440-43-9	4.17E+03		1.50E+01		1.50E+01		6.00E+01	
calcium	7440-70-2	4.17E+03		1.50E+01		1.50E+01		6.00E+01	
carbon dioxide (CO2)	124-38-9	4.17E+03	180	1.50E+01	15	1.50E+01	30	6.00E+01	140
carbon disulfide	75-15-0	4.17E+03	180	1.50E+01	15	1.50E+01	30	6.00E+01	140
carbon monoxide (CO)	630-08-0	1.56E-01	2	1.50E+01	15	1.50E+01	30	6.00E+01	140
carbon tetrachloride	56-23-5	4.17E+03	180	6.00E+01	60	6.00E+01	120	2.40E+02	540
carbonyl sulfide	463-58-1	4.17E+03	180	1.50E+01	15	1.50E+01	30	6.00E+01	140
chlorobenzene	108-90-7	1.39E+01	21	1.50E+01	15	1.50E+01	30	6.00E+01	140
chloroethene (vinyl chloride)	75-01-4	1.49E+00	2.2	1.50E+01	15	1.50E+01	30	6.00E+01	140
chloroform	67-66-3	1.04E+02	150	3.75E+01	38	3.75E+01	75	1.50E+02	340
chloromethane	74-87-3	2.45E+02	370	1.50E+01	15	1.50E+01	30	6.00E+01	140
chromium	7440-47-3	4.17E+03		1.50E+01		1.50E+01		6.00E+01	
chrysene	218-01-9	2.14E-01	0.32	6.00E+01	60	6.00E+01	120	2.40E+02	540

Table 23 (Continued)

Chemical	CAS Number	Half-Life, days							
		Air		Water		Soil		Sediment	
		EPI	PBT	EPI	PBT	EPI	PBT	EPI	PBT
cis-2-butene	590-18-1	5.77E-02	0.04	8.67E+00	8.7	8.67E+00	17	3.47E+01	78
Cl2 (a)	7782-50-5	4.17E+03	180	1.50E+01	15	1.50E+01	30	6.00E+01	140
cobalt	7440-48-4	4.17E+03		1.50E+01		1.50E+01		6.00E+01	
copper	7440-50-8	4.17E+03		1.50E+01		1.50E+01		6.00E+01	
dibenz(a,h)anthracene	53-70-3	2.14E-01	0.32	6.00E+01	60	6.00E+01	120	2.40E+02	540
dibenzo(b,def)chrysene-7,14 dione (c.i. vat yellow 4)	128-66-5	6.49E-01	0.96	3.75E+01	38	3.75E+01	75	1.50E+02	340
dibutyl phthalate	84-74-2	1.15E+00	1.8	8.67E+00	8.7	8.67E+00	17	3.47E+01	78
dichloroacetonitrile	3018-12-0	2.01E+02	300	3.75E+01	38	3.75E+01	75	1.50E+02	340
dichlorodiflouromethane	75-71-8	4.17E+03	180	3.75E+01	38	3.75E+01	75	1.50E+02	340
dimethyltrisulfide	3658-80-8	2.37E-02	0.03	1.50E+01	15	1.50E+01	30	6.00E+01	140
diphenylamine	122-39-4	5.51E-02	0.08	3.75E+01	38	3.75E+01	75	1.50E+02	340
ethane	74-84-0	3.99E+01	58	1.50E+01	15	1.50E+01	30	6.00E+01	140
ethanol	64-17-5	3.27E+00	5	8.67E+00	8.7	8.67E+00	17	3.47E+01	78
ethyl benzene	100-41-4	1.51E+00	2.2	1.50E+01	15	1.50E+01	30	6.00E+01	140
ethyl chloride	75-00-3	2.60E+01	39	1.50E+01	15	1.50E+01	30	6.00E+01	140
ethylene	74-85-1	1.05E+00	1.5	1.50E+01	15	1.50E+01	30	6.00E+01	140
fluoranthene	206-44-0	9.73E-01	1.5	6.00E+01	60	6.00E+01	120	2.40E+02	540
fluorene	86-73-7	8.23E-01	1.2	1.50E+01	15	1.50E+01	30	6.00E+01	140
formaldehyde	50-00-0	1.14E+00	1.7	1.50E+01	15	1.50E+01	30	6.00E+01	140
furan	110-00-9	2.50E-01	0.37	1.50E+01	15	1.50E+01	30	6.00E+01	140
HCl	7647-01-0	4.17E+03		1.50E+01		1.50E+01		6.00E+01	
heptanal	111-71-7	3.54E-01	0.54	8.67E+00	8.7	8.67E+00	17	3.47E+01	78
hexachlorobenzene	118-74-1	3.96E+01	58	1.50E+02	180	1.50E+02	360	6.00E+02	1

(Sheet 5 of 8)

Table 23 (Continued)

Chemical	CAS Number	Half-Life, days							
		Air		Water		Soil		Sediment	
		EPI	PBT	EPI	PBT	EPI	PBT	EPI	PBT
hexachlorobutadiene	87-68-3	3.56E+02	540	1.50E+02	180	1.50E+02	360	6.00E+02	1
hexachlorocyclopentadiene	77-47-4	2.70E+01	40	1.50E+02	180	1.50E+02	360	6.00E+02	1
hexachloroethane	67-72-1	4.17E+03	180	1.50E+02	180	1.50E+02	360	6.00E+02	1
hexanal	66-25-1	3.37E-01	0.5	8.67E+00	8.7	8.67E+00	17	3.47E+01	78
hexane	110-54-3	1.91E+00	2.9	8.67E+00	8.7	8.67E+00	17	3.47E+01	78
HMX	2691-41-0	3.26E-02	0.05	3.75E+01	38	3.75E+01	75	1.50E+02	340
hydrogen cyanide	74-90-8	3.57E+02	540	1.50E+01	15	1.50E+01	30	6.00E+01	140
i-butane (isobutane)	75-28-5	4.57E+00	6.7	1.50E+01	15	1.50E+01	30	6.00E+01	140
i-butene (isobutene/e-butylene)	115-11-7	1.71E-01	0.23	1.50E+01	15	1.50E+01	30	6.00E+01	140
indeno(1,2,3-cd)pyrene	193-39-5	1.66E-01	0.25	6.00E+01	60	6.00E+01	120	2.40E+02	540
isothiocyanatomethane	556-61-6	7.87E+01	120	1.50E+01	15	1.50E+01	30	6.00E+01	140
lead	7439-92-1	4.17E+03		3.75E+01		3.75E+01		1.50E+02	
xylene (mixed isomers)	1330-20-7	7.81E-01	1.2	1.50E+01	15	1.50E+01	30	6.00E+01	140
m-xylene (meta-xylene)	108-38-3	4.53E-01	0.67	1.50E+01	15	1.50E+01	30	6.00E+01	140
p-xylene (para-xylene)	106-42-3	7.48E-01	1.1	1.50E+01	15	1.50E+01	30	6.00E+01	140
magnesium	7439-95-4	4.17E+03		1.50E+01		1.50E+01		6.00E+01	
manganese	7439-96-5	4.17E+03		1.50E+01		1.50E+01		6.00E+01	
m-dichlorobenzene	541-73-1	1.49E+01	22	3.75E+01	38	3.75E+01	75	1.50E+02	340
mercury	7439-97-6	4.17E+03		1.50E+01		1.50E+01		6.00E+01	
methacrolein	78-85-3	3.10E-01	0.46	1.50E+01	15	1.50E+01	30	6.00E+01	140
methane	74-82-8	1.56E-01	2	1.50E+01	15	1.50E+01	30	6.00E+01	140
methylene chloride	75-09-2	7.53E+01	110	3.75E+01	38	3.75E+01	75	1.50E+02	340
methylnitrite	624-91-9	4.61E+01	67	1.50E+01	15	1.50E+01	30	6.00E+01	140
methyl-t-butylether (MTBE)	1634-04-4	3.64E+00	5.4	1.50E+01	15	1.50E+01	30	6.00E+01	140

Table 23 (Continued)

Chemical	CAS Number	Half-Life, days							
		Air		Water		Soil		Sediment	
		EPI	PBT	EPI	PBT	EPI	PBT	EPI	PBT
methyl-vinyl ketone	78-94-4	4.60E-01	0.62	1.50E+01	15	1.50E+01	30	6.00E+01	140
naphthalene	91-20-3	4.95E-01	0.75	3.75E+01	38	3.75E+01	75	1.50E+02	340
n-butane	106-97-8	4.21E+00	6.2	8.67E+00	8.7	8.67E+00	17	3.47E+01	78
n-decane	124-18-5	9.22E-01	1.4	8.67E+00	8.7	8.67E+00	17	3.47E+01	78
NH3 (ammonia)	7664-41-7	4.17E+03		1.50E+01		1.50E+01		6.00E+01	
nickel	7440-02-0	4.17E+03		1.50E+01		1.50E+01		6.00E+01	
nitric acid	7697-37-2	2.97E+01		1.50E+01		1.50E+01		6.00E+01	
nitrobenzene	98-95-3	7.64E+01	120	1.50E+01	15	1.50E+01	30	6.00E+01	140
nitrogen oxide (NOx)	10102-44-0	8.23E+01		1.50E+01		1.50E+01		6.00E+01	
nitroglycerine	55-63-0	9.74E+00	15	3.75E+01	38	3.75E+01	75	1.50E+02	340
nitromethane	75-52-5	8.23E+01	120	1.50E+01	15	1.50E+01	30	6.00E+01	140
nonanal	124-19-6	3.23E-01	0.5	1.50E+01	15	1.50E+01	30	6.00E+01	140
OCDD (1,2,3,4,6,7,8,9-OCDD)	3268-87-9	1.97E+02	300	1.50E+02	180	1.50E+02	360	6.00E+02	1
octanal	124-13-0	3.38E-01	0.5	1.50E+01	15	1.50E+01	30	6.00E+01	140
o-dichlorobenzene	95-50-1	2.55E+01	38	3.75E+01	38	3.75E+01	75	1.50E+02	340
o-methoxy-phenyl-azo-b-naphthol (oil red g)	1229-55-6	3.98E-01	0.58	3.75E+01	38	3.75E+01	75	1.50E+02	340
o-xylene (ortho-xylene)	95-47-6	7.81E-01	1.2	1.50E+01	15	1.50E+01	30	6.00E+01	140
particulate cyanide	57-12-5	3.57E+02	540	1.50E+01	15	1.50E+01	30	6.00E+01	140
p-dichlorobenzene (para-dichlorobenzene)	106-46-7	3.34E+01	50	3.75E+01	38	3.75E+01	75	1.50E+02	340
pentaerythritoltetranitrate (PETN)	78-11-5	6.59E+00	10	3.75E+01	38	3.75E+01	75	1.50E+02	340
perchloroethylene	127-18-4	6.38E+01	96	6.00E+01	60	6.00E+01	120	2.40E+02	540
phenanthrene	85-01-8	8.23E-01	1.2	6.00E+01	60	6.00E+01	120	2.40E+02	540
phenol	108-95-2	4.07E-01	0.62	1.50E+01	15	1.50E+01	30	6.00E+01	140
phenylacetylene (ethynyl benzene)	536-74-3	1.28E+00	1.9	1.50E+01	15	1.50E+01	30	6.00E+01	140

(Sheet 7 of 8)

Table 23 (Concluded)

Chemical	CAS Number	Half-Life, days							
		Air		Water		Soil		Sediment	
		EPI	PBT	EPI	PBT	EPI	PBT	EPI	PBT
phosphorus	7723-14-0	4.17E+03		1.50E+01		1.50E+01		6.00E+01	
propanal	123-38-6	5.46E-01	0.83	1.50E+01	15	1.50E+01	30	6.00E+01	140
propane	74-98-6	9.30E+00	14	1.50E+01	15	1.50E+01	30	6.00E+01	140
propylene	115-07-1	2.90E-01	0.38	1.50E+01	15	1.50E+01	30	6.00E+01	140
propyne	74-99-7	1.81E+00	2.7	1.50E+01	15	1.50E+01	30	6.00E+01	140
pyrene	129-00-0	2.14E-01	0.32	6.00E+01	60	6.00E+01	120	2.40E+02	540
RDX	121-82-4	4.35E-02	0.06	3.75E+01	38	3.75E+01	75	1.50E+02	340
selenium	7782-49-2	1.65E-01		1.50E+01		1.50E+01		6.00E+01	
silver	7440-22-4	4.17E+03		1.50E+01		1.50E+01		6.00E+01	
styrene (vinyl benzene)	100-42-5	1.37E-01	0.18	1.50E+01	15	1.50E+01	30	6.00E+01	140
sulfur dioxide (SO2)	7446 09 5	1.78E-01		1.50E+01		1.50E+01		6.00E+01	
sulfuric acid	7664-93-9	3.82E+01		1.50E+01		1.50E+01		6.00E+01	
tetryl (2,4,6-trinitrophenylmethylnitramine)	479-45-8	8.45E+00	12	6.00E+01	60	6.00E+01	120	2.40E+02	540
thallium	7440-28-0	4.17E+03		3.75E+01		3.75E+01		1.50E+02	
thiophene	110-02-1	1.12E+00	1.7	1.50E+01	15	1.50E+01	30	6.00E+01	140
toluene	108-88-3	1.79E+00	2.7	1.50E+01	15	1.50E+01	30	6.00E+01	140
trans-2-butenal	123-73-9	2.84E-01	0.42	1.50E+01	15	1.50E+01	30	6.00E+01	140
trans-2-butene	624-64-6	5.77E-02	0.04	8.67E+00	8.7	8.67E+00	17	3.47E+01	78
trans-2-pentene	646-04-8	2.96E-02	0.04	8.67E+00	8.7	8.67E+00	17	3.47E+01	78
trans-3-penten-2-one	625-33-2	1.51E-01	0.2	1.50E+01	15	1.50E+01	30	6.00E+01	140
trichloroethylene (TCE)	79-01-6	4.52E+00	6.7	3.75E+01	38	3.75E+01	75	1.50E+02	340
trichloroflouromethane	75-69-4	4.17E+03	180	6.00E+01	60	6.00E+01	120	2.40E+02	540
vinylidenechloride	75-35-4	9.81E-01	1.5	3.75E+01	38	3.75E+01	75	1.50E+02	340
zinc	7440-66-6	4.17E+03		1.50E+01		1.50E+01		6.00E+01	

Table 24
EPI Half-Life (days)

Chemical	CAS Number	Air[1]	Surface Water[1]	Soil[1]	Sediment[1]	Oxidation in Air	Biodegradation	
							Water	Soil
1,2-dichloroethene (cis)	156-59-2	4.11E+00	3.75E+01	3.75E+01	1.50E+02	4.30E+00	2.01E+01	6.43E+00
1,2-dichloroethene (trans)	156-60-5	4.11E+00	3.75E+01	3.75E+01	1.50E+02	3.79E+00	2.01E+01	6.43E+00
(1,2-dichloroethyl) benzene	1074-11-9	4.45E+00	3.75E+01	3.75E+01	1.50E+02	4.45E+00	2.26E+02	7.66E+00
1,2,4-trimethylbenzene	95-63-6	3.29E-01	3.75E+01	3.75E+01	1.50E+02	6.41E-01	2.63E+02	6.84E+00
1,2-dichlorethane	107-06-2	4.31E+01	3.75E+01	3.75E+01	1.50E+02	4.19E+01	5.62E+00	6.47E+00
1,2-dichloro-3-methylbenzene	32768-54-0	9.05E+00	3.75E+01	3.75E+01	1.50E+02	9.05E+00	3.27E+02	1.03E+01
1,2-dichloroethene (cis/trans mixture)	540-59-0	4.11E+00	3.75E+01	3.75E+01	1.50E+02	4.30E+00	2.01E+01	6.43E+00
1,3,5-trimethylbenzene (mesitylene)	108-67-8	1.86E-01	3.75E+01	3.75E+01	1.50E+02	3.05E-01	2.14E+02	6.84E+00
1,3,5-trinitrobenzene	99-35-4	8.23E+03	6.00E+01	6.00E+01	2.40E+02	8.22E+03	3.17E+00	1.03E+01
1,3-butadiene	106-99-0	1.44E-01	1.50E+01	1.50E+01	6.00E+01	1.61E-01	1.63E+01	4.21E+00
1,3-dinitrobenzene	99-65-0	3.51E+02	3.75E+01	3.75E+01	1.50E+02	3.51E+02	5.74E+00	7.79E+00
1,4-diamino-2,3-dihydroanthraquinone (DDA) violet-dye mix	81-63-0	6.20E-02	3.75E+01	3.75E+01	1.50E+02	1.03E-01	1.24E+00	6.10E+00
1,4-di-p-toluidinoanthraquinone (PTA) solvent green 3	128-80-3	5.34E-02	6.00E+01	6.00E+01	2.40E+02	5.30E-02	4.17E+02	1.87E+01
1-butanol	71-36-3	1.25E+00	8.67E+00	8.67E+00	3.47E+01	1.55E+00	1.92E+00	2.32E+00
1-butene	106-98-9	2.57E-01	8.67E+00	8.67E+00	3.47E+01	3.90E-01	3.86E+01	2.74E+00
1-chloro-2-methylbenzene	95-49-8	5.88E+00	3.75E+01	3.75E+01	1.50E+02	5.89E+00	2.14E+02	7.27E+00
1-chloro-3-methylbenzene	108-41-8	2.88E+00	3.75E+01	3.75E+01	1.50E+02	2.88E+00	1.80E+02	7.27E+00
1-hexene	592-41-6	2.21E-01	8.67E+00	8.67E+00	3.47E+01	3.54E-01	2.07E+02	2.92E+00
1-pentene	109-67-1	2.59E-01	8.67E+00	8.67E+00	3.47E+01	3.72E-01	6.49E+01	2.83E+00
1-(methylamino)anthraquinone (disperse red 9)	82-38-2	5.81E-01	3.75E+01	3.75E+01	1.50E+02	5.81E-01	3.48E+02	8.25E+00
2-(2-quinolyl)-1,3-indandione (D & C yellow no. 11) or (solvent yellow 33)	8003-22-3	3.69E-01	3.75E+01	3.75E+01	1.50E+02	3.69E-01	3.48E+02	8.41E+00
2,3-butanedione	431-03-8	4.50E+01	1.50E+01	1.50E+01	6.00E+01	5.24E+01	6.73E-01	4.54E+00
2,3,7,8-tetrachlorodibenzo-p-dioxin	1746-01-6	1.42E+01	1.50E+02	1.50E+02	6.00E+02	1.42E+01	4.17E+02	1.78E+01
2,4,6-trinitrotoluene (TNT)	118-96-7	7.78E+01	6.00E+01	6.00E+01	2.40E+02	7.77E+01	7.18E+00	1.19E+01

(Sheet 1 of 7)

[1] Values are the same as those in Table 23 for EPI.

Table 24 (Continued)

Chemical	CAS Number	Air[1]	Surface Water[1]	Soil[1]	Sediment[1]	Oxidation in Air	Biodegradation	
							Water	Soil
2,6-dinitrotoluene (2,6-DNT)	606-20-2	4.96E+01	3.75E+01	3.75E+01	1.50E+02	4.96E+01	2.06E+01	8.99E+00
2,5-dimethylfuran	625-86-5	8.10E-02	1.50E+01	1.50E+01	6.00E+01	8.20E-02	2.77E+01	5.79E+00
2-amino-4,6-dinitrotoluene	35572-78-2	9.35E+00	6.00E+01	6.00E+01	2.40E+02	9.35E+00	1.19E+01	1.11E+01
2-amino-9,10-anthracenedione (a) (AAQ)	117-79-3	2.54E-01	3.75E+01	3.75E+01	1.50E+02	2.54E-01	4.10E+01	7.99E+00
2-butanone	78-93-3	9.30E+00	1.50E+01	1.50E+01	6.00E+01	8.03E+00	9.89E-01	4.55E+00
2-furaldehyde	98-01-1	3.05E-01	1.50E+01	1.50E+01	6.00E+01	2.86E-01	1.09E+00	3.38E+00
2-heptanone	110-43-0	9.14E-01	1.50E+01	1.50E+01	6.00E+01	1.31E+00	1.59E+01	3.25E+00
2-methyl-1-butene	563-46-2	1.48E-01	1.50E+01	1.50E+01	6.00E+01	2.03E-01	7.27E+01	4.37E+00
2-methylfuran	534-22-5	1.73E-01	1.50E+01	1.50E+01	6.00E+01	1.01E-01	1.21E+01	5.02E+00
2-methylthiophene	554-14-3	4.28E-01	1.50E+01	1.50E+01	6.00E+01	4.28E-01	3.34E+01	5.21E+00
2-nitrotoluene (ONT)	88-72-2	1.53E+01	3.75E+01	3.75E+01	1.50E+02	1.39E+01	3.14E+01	6.79E+00
2-pentanone	107-87-9	2.30E+00	1.50E+01	1.50E+01	6.00E+01	2.24E+00	2.01E+00	4.70E+00
2-propanol	67-63-0	2.11E+00	1.50E+01	1.50E+01	6.00E+01	1.47E+00	8.52E-01	3.46E+00
2-thiophenecarboxaldehyde	98-03-3	4.93E-01	1.50E+01	1.50E+01	6.00E+01	4.93E-01	2.40E+00	3.51E+00
3-(phenylhydrazone)-1H-indole-2,3-dione	17310-26-8	1.86E-01	3.75E+01	3.75E+01	1.50E+02	1.86E-01	3.63E+01	4.59E+00
3-furaldehyde	498-60-2	2.21E-01	1.50E+01	1.50E+01	6.00E+01	2.86E-01	1.20E+00	3.38E+00
3-methyl-1-butene	563-45-1	2.63E-01	1.50E+01	1.50E+01	6.00E+01	3.74E-01	5.66E+01	4.37E+00
3-methylfuran	930-27-8	1.14E-01	1.50E+01	1.50E+01	6.00E+01	1.01E-01	1.37E+01	5.02E+00
3-methylthiophene	616-44-4	4.28E-01	1.50E+01	1.50E+01	6.00E+01	4.28E-01	3.41E+01	5.21E+00
3-nitrotoluene	99-08-1	1.13E+01	3.75E+01	3.75E+01	1.50E+02	1.84E+01	4.28E+01	6.79E+00
4-1,2,4-oxadizaolin-3-one-2,5-diphenyl-delta		6.40E-01	3.75E+01	3.75E+01	1.50E+02	6.40E-01	8.44E+01	6.36E+00
4-amino-2,6-dinitrotoluene (4ADNT)	19406-51-0	9.35E+00	6.00E+01	6.00E+01	2.40E+02	9.35E+00	1.19E+01	1.11E+01
4-ethyltoluene	622-96-8	8.84E-01	1.50E+01	1.50E+01	6.00E+01	1.44E+00	2.63E+02	6.12E+00
4-methyl-2-pentanone	108-10-1	7.59E-01	1.50E+01	1.50E+01	6.00E+01	1.21E+00	4.03E+00	4.86E+00
4-nitrotoluene	99-99-0	1.39E+01	3.75E+01	3.75E+01	1.50E+02	1.39E+01	3.63E+01	6.79E+00
4-phenoxy-2(1H)-quinolinone	66662-28-0	5.63E-02	3.75E+01	3.75E+01	1.50E+02	1.16E-01	6.00E+01	4.05E+00
acenaphthene	83-32-9	1.84E-01	3.75E+01	3.75E+01	1.50E+02	1.60E-01	3.20E+02	6.63E+00

Table 24 (Continued)

Chemical	CAS Number	Air[1]	Surface Water[1]	Soil[1]	Sediment[1]	Oxidation in Air	Biodegradation	
							Water	Soil
acenaphthylene	208-96-8	3.10E-02	1.50E+01	1.50E+01	6.00E+01	1.42E-01	3.24E+02	5.29E+00
acetaldehyde	75-07-0	6.77E-01	1.50E+01	1.50E+01	6.00E+01	6.30E-01	7.42E-01	2.99E+00
acetic acid	64-19-7	1.45E+01	8.67E+00	8.67E+00	3.47E+01	1.72E+01	7.78E-01	2.29E+00
acetone	67-64-1	4.88E+01	1.50E+01	1.50E+01	6.00E+01	5.24E+01	7.61E-01	4.40E+00
acetonitrile	75-05-8	6.43E+01	1.50E+01	1.50E+01	6.00E+01	4.14E+02	7.42E-01	4.54E+00
acetophenone	98-86-2	3.90E+00	1.50E+01	1.50E+01	6.00E+01	5.69E+00	6.89E+00	5.05E+00
acetylene	74-86-2	1.24E+01	1.50E+01	1.50E+01	6.00E+01	1.31E+01	1.05E+00	3.94E+00
acrolein	107-02-8	5.30E-01	1.50E+01	1.50E+01	6.00E+01	4.14E-01	8.28E-01	3.08E+00
acrylonitrile	107-13-1	2.56E+00	1.50E+01	1.50E+01	6.00E+01	2.54E+00	9.61E-01	4.67E+00
aluminum	7429-90-5	4.17E+03	1.50E+01	1.50E+01	6.00E+01	1.00E+06	1.02E+00	3.98E+00
anthracene	120-12-7	2.67E-01	6.00E+01	6.00E+01	2.40E+02	2.67E-01	3.83E+02	9.77E+00
antimony	7440-36-0	4.17E+03	1.50E+01	1.50E+01	6.00E+01	1.00E+06	1.56E+00	4.96E+00
arsenic	7440-38-2	4.17E+03	1.50E+01	1.50E+01	6.00E+01	1.00E+06	1.46E+00	4.45E+00
barium	7440-39-3	4.17E+03	1.50E+01	1.50E+01	6.00E+01	1.00E+06	9.48E-01	5.11E+00
benzaldehyde	100-52-7	8.29E-01	1.50E+01	1.50E+01	6.00E+01	5.99E-01	5.62E+00	3.43E+00
benzanthrone (b)	82-05-3	5.94E-01	3.75E+01	3.75E+01	1.50E+02	5.94E-01	4.01E+02	6.58E+00
benzene	71-43-2	8.70E+00	3.75E+01	3.75E+01	1.50E+02	5.49E+00	2.19E+01	7.74E+00
benzo(a)anthracene	56-55-3	2.14E-01	6.00E+01	6.00E+01	2.40E+02	2.14E-01	4.15E+02	1.96E+01
benzo(a)pyrene	50-32-8	2.14E-01	6.00E+01	6.00E+01	2.40E+02	2.14E-01	4.16E+02	2.07E+01
benzo(b)fluoranthene	205-99-2	5.77E-01	6.00E+01	6.00E+01	2.40E+02	5.76E-01	4.15E+02	2.07E+01
benzo(e)pyrene	192-97-2	2.14E-01	6.00E+01	6.00E+01	2.40E+02	2.14E-01	4.16E+02	2.07E+01
benzo(g,h,i)perylene	191-24-2	1.23E-01	6.00E+01	6.00E+01	2.40E+02	1.23E-01	4.16E+02	2.19E+01
benzo(k)fluoranthene	207-08-9	2.00E-01	6.00E+01	6.00E+01	2.40E+02	1.99E-01	4.16E+02	2.07E+01
benzofuran	271-89-6	2.87E-01	1.50E+01	1.50E+01	6.00E+01	2.87E-01	6.61E+01	4.89E+00
benzonitrile	100-47-0	3.24E+01	1.50E+01	1.50E+01	6.00E+01	3.11E+01	6.61E+00	5.20E+00
beryllium	7440-41-7	4.17E+03	1.50E+01	1.50E+01	6.00E+01	1.00E+06	7.10E-01	3.79E+00
bis(2-ethylhexyl)phthalate	117-81-7	4.87E-01	1.50E+01	1.50E+01	6.00E+01	4.87E-01	4.17E+02	1.85E+00
butanal	123-72-8	4.55E-01	1.50E+01	1.50E+01	6.00E+01	4.21E-01	1.92E+00	3.20E+00
cadmium	7440-43-9	4.17E+03	1.50E+01	1.50E+01	6.00E+01	1.00E+06	8.07E-01	4.82E+00
calcium	7440-70-2	4.17E+03	1.50E+01	1.50E+01	6.00E+01	1.00E+06	7.10E-01	4.09E+00

(Sheet 3 of 7)

Table 24 (Continued)

Chemical	CAS Number	Air[1]	Surface Water[1]	Soil[1]	Sediment[1]	Oxidation in Air	Biodegradation	
							Water	Soil
carbon dioxide (CO2)	124-38-9	4.17E+03	1.50E+01	1.50E+01	6.00E+01	1.00E+06	1.79E+00	4.11E+00
carbon disulfide	75-15-0	4.17E+03	1.50E+01	1.50E+01	6.00E+01	1.00E+06	1.46E+01	4.43E+00
carbon monoxide (CO)	630-08-0	1.56E-01	1.50E+01	1.50E+01	6.00E+01	1.56E+03	1.04E+01	3.97E+00
carbon tetrachloride	56-23-5	4.17E+03	6.00E+01	6.00E+01	2.40E+02	1.00E+06	8.91E+01	1.30E+01
carbonyl sulfide	463-58-1	4.17E+03	1.50E+01	1.50E+01	6.00E+01	1.00E+06	6.73E-01	4.27E+00
chlorobenzene	108-90-7	1.39E+01	1.50E+01	1.50E+01	6.00E+01	7.80E+00	9.07E+01	6.25E+00
chloroethene (vinyl chloride)	75-01-4	1.49E+00	1.50E+01	1.50E+01	6.00E+01	1.94E+00	7.48E+00	5.05E+00
chloroform	67-66-3	1.04E+02	3.75E+01	3.75E+01	1.50E+02	1.00E+02	1.56E+01	7.98E+00
chloromethane	74-87-3	2.45E+02	1.50E+01	1.50E+01	6.00E+01	2.07E+02	2.01E+00	4.91E+00
chromium	7440-47-3	4.17E+03	1.50E+01	1.50E+01	6.00E+01	1.00E+06	9.48E-01	4.19E+00
chrysene	218-01-9	2.14E-01	6.00E+01	6.00E+01	2.40E+02	2.14E-01	4.15E+02	1.96E+01
cis-2-butene	590-18-1	5.77E-02	8.67E+00	8.67E+00	3.47E+01	2.27E+00	3.20E+01	2.74E+00
Cl2 (a)	7782-50-5	4.17E+03	1.50E+01	1.50E+01	6.00E+01	1.00E+06	1.84E+00	4.38E+00
cobalt	7440-48-4	4.17E+03	1.50E+01	1.50E+01	6.00E+01	1.00E+06	9.48E-01	4.26E+00
copper	7440-50-8	4.17E+03	1.50E+01	1.50E+01	6.00E+01	1.00E+06	7.10E-01	4.30E+00
dibenz(a,h)anthracene	53-70-3	2.14E-01	6.00E+01	6.00E+01	2.40E+02	2.14E-01	4.16E+02	2.20E+01
dibenzo(b,def)chrysene-7,14 dione (c.i. vat yellow 4)	128-66-5	6.49E-01	3.75E+01	3.75E+01	1.50E+02	6.49E-01	4.16E+02	8.64E+00
dibutyl phthalate	84-74-2	1.15E+00	8.67E+00	8.67E+00	3.47E+01	1.15E+00	3.86E+02	1.42E+00
dichloroacetonitrile	3018-12-0	2.01E+02	3.75E+01	3.75E+01	1.50E+02	2.01E+02	9.89E-01	7.37E+00
dichlorodiflouromethane	75-71-8	4.17E+03	3.75E+01	3.75E+01	1.50E+02	1.00E+06	2.34E+01	8.72E+00
dimethyltrisulfide	3658-80-8	2.37E-02	1.50E+01	1.50E+01	6.00E+01	2.40E-02	1.26E+01	4.98E+00
diphenylamine	122-39-4	5.51E-02	3.75E+01	3.75E+01	1.50E+02	5.30E-02	2.33E+02	6.45E+00
ethane	74-84-0	3.99E+01	1.50E+01	1.50E+01	6.00E+01	3.93E+01	1.11E+01	3.98E+00
ethanol	64-17-5	3.27E+00	8.67E+00	8.67E+00	3.47E+01	2.99E+00	7.47E-01	3.35E+00
ethyl benzene	100-41-4	1.51E+00	1.50E+01	1.50E+01	6.00E+01	1.80E+00	1.51E+02	5.27E+00
ethyl chloride	75-00-3	2.60E+01	1.50E+01	1.50E+01	6.00E+01	2.65E+01	5.09E+00	5.07E+00
ethylene	74-85-1	1.05E+00	1.50E+01	1.50E+01	6.00E+01	1.26E+00	2.89E+00	3.96E+00
fluoranthene	206-44-0	9.73E-01	6.00E+01	6.00E+01	2.40E+02	3.66E-01	4.10E+02	1.85E+01
fluorene	86-73-7	8.23E-01	1.50E+01	1.50E+01	6.00E+01	1.21E+00	3.58E+02	6.10E+00

Table 24 (Continued)

Chemical	CAS Number	Air[1]	Surface Water[1]	Soil[1]	Sediment[1]	Oxidation in Air	Biodegradation	
							Water	Soil
formaldehyde	50-00-0	1.14E+00	1.50E+01	1.50E+01	6.00E+01	1.32E+00	1.04E+00	2.90E+00
furan	110-00-9	2.50E-01	1.50E+01	1.50E+01	6.00E+01	2.64E-01	4.27E+00	4.35E+00
HCl	7647-01-0	4.17E+03	1.50E+01	1.50E+01	6.00E+01	1.00E+06	1.24E+00	4.03E+00
heptanal	111-71-7	3.54E-01	8.67E+00	8.67E+00	3.47E+01	3.54E-01	3.07E+01	2.28E+00
hexachlorobenzene	118-74-1	3.96E+01	1.50E+02	1.50E+02	6.00E+02	6.33E+02	4.15E+02	3.57E+01
hexachlorobutadiene	87-68-3	3.56E+02	1.50E+02	1.50E+02	6.00E+02	3.56E+02	4.00E+02	1.80E+01
hexachlorocyclopentadiene	77-47-4	2.70E+01	1.50E+02	1.50E+02	6.00E+02	2.72E+01	4.07E+02	2.38E+01
hexachloroethane	67-72-1	4.17E+03	1.50E+02	1.50E+02	6.00E+02	1.00E+06	3.53E+02	2.80E+01
hexanal	66-25-1	3.37E-01	8.67E+00	8.67E+00	3.47E+01	3.71E-01	1.04E+01	2.21E+00
hexane	110-54-3	1.91E+00	8.67E+00	8.67E+00	3.47E+01	1.96E+00	3.17E+02	2.94E+00
HMX	2691-41-0	3.26E-02	3.75E+01	3.75E+01	1.50E+02	3.30E-02	1.76E+00	7.39E+00
hydrogen cyanide	74-90-8	3.57E+02	1.50E+01	1.50E+01	6.00E+01	3.57E+02	7.59E-01	3.95E+00
i-butane (isobutane)	75-28-5	4.57E+00	1.50E+01	1.50E+01	6.00E+01	4.38E+00	7.84E+01	4.25E+00
i-butene (isobutene/e-butylene)	115-11-7	1.71E-01	1.50E+01	1.50E+01	6.00E+01	2.07E-01	3.41E+01	4.23E+00
indeno(1,2,3-cd)pyrene	193-39-5	1.66E-01	6.00E+01	6.00E+01	2.40E+02	1.66E-01	4.16E+02	2.19E+01
isothiocyanatomethane	556-61-6	7.87E+01	1.50E+01	1.50E+01	6.00E+01	7.86E+01	2.11E+00	4.40E+00
lead	7439-92-1	4.17E+03	3.75E+01	3.75E+01	1.50E+02	1.00E+06	1.56E+00	6.01E+00
xylene (mixed isomers)	1330-20-7	7.81E-01	1.50E+01	1.50E+01	6.00E+01	1.64E+00	1.44E+02	5.93E+00
m-xylene (meta-xylene)	108-38-3	4.53E-01	1.50E+01	1.50E+01	6.00E+01	7.89E-01	1.62E+02	5.93E+00
p-xylene (para-xylene)	106-42-3	7.48E-01	1.50E+01	1.50E+01	6.00E+01	1.64E+00	1.51E+02	5.93E+00
magnesium	7439-95-4	4.17E+03	1.50E+01	1.50E+01	6.00E+01	1.00E+06	7.10E-01	3.95E+00
manganese	7439-96-5	4.17E+03	1.50E+01	1.50E+01	6.00E+01	1.00E+06	9.48E-01	4.22E+00
m-dichlorobenzene	541-73-1	1.49E+01	3.75E+01	3.75E+01	1.50E+02	1.11E+01	2.40E+02	8.91E+00
mercury	7439-97-6	4.17E+03	1.50E+01	1.50E+01	6.00E+01	1.00E+06	1.36E+00	5.92E+00
methacrolein	78-85-3	3.10E-01	1.50E+01	1.50E+01	6.00E+01	3.10E-01	1.58E+00	3.18E+00
methane	74-82-8	1.56E-01	1.50E+01	1.50E+01	6.00E+01	1.56E+03	2.70E+00	3.85E+00
methylene chloride	75-09-2	7.53E+01	3.75E+01	3.75E+01	1.50E+02	7.93E+01	3.60E+00	6.26E+00
methylnitrite	624-91-9	4.61E+01	1.50E+01	1.50E+01	6.00E+01	6.92E+01	1.92E+00	4.28E+00
methyl-t-butylether (MTBE)	1634-04-4	3.64E+00	1.50E+01	1.50E+01	6.00E+01	4.74E+00	2.11E+00	5.93E+00
methyl-vinyl ketone	78-94-4	4.60E-01	1.50E+01	1.50E+01	6.00E+01	4.50E-01	1.09E+00	4.53E+00

(Sheet 5 of 7)

Table 24 (Continued)

Chemical	CAS Number	Air[1]	Surface Water[1]	Soil[1]	Sediment[1]	Oxidation in Air	Biodegradation	
							Water	Soil
naphthalene	91-20-3	4.95E-01	3.75E+01	3.75E+01	1.50E+02	4.95E-01	1.85E+02	8.70E+00
n-butane	106-97-8	4.21E+00	8.67E+00	8.67E+00	3.47E+01	4.06E+00	9.91E+01	2.75E+00
n-decane	124-18-5	9.22E-01	8.67E+00	8.67E+00	3.47E+01	9.63E-01	4.07E+02	2.17E+00
NH3 (ammonia)	7664-41-7	4.17E+03	1.50E+01	1.50E+01	6.00E+01	1.00E+06	6.73E-01	3.86E+00
nickel	7440-02-0	4.17E+03	1.50E+01	1.50E+01	6.00E+01	1.00E+06	7.10E-01	4.25E+00
nitric acid	7697-37-2	2.97E+01	1.50E+01	1.50E+01	6.00E+01	2.97E+01	9.35E-01	4.29E+00
nitrobenzene	98-95-3	7.64E+01	1.50E+01	1.50E+01	6.00E+01	4.39E+01	1.21E+01	5.84E+00
nitrogen oxide (NOx)	10102-44-0	8.23E+01	1.50E+01	1.50E+01	6.00E+01	8.23E+01	7.09E-01	4.13E+00
nitroglycerine	55-63-0	9.74E+00	3.75E+01	3.75E+01	1.50E+02	9.74E+00	7.48E+00	6.30E+00
nitromethane	75-52-5	8.23E+01	1.50E+01	1.50E+01	6.00E+01	8.23E+01	7.40E-01	4.28E+00
nonanal	124-19-6	3.23E-01	1.50E+01	1.50E+01	6.00E+01	3.23E-01	1.78E+02	2.44E+00
OCDD (1,2,3,4,6,7,8,9-OCDD)	3268-87-9	1.97E+02	1.50E+02	1.50E+02	6.00E+02	1.97E+02	4.17E+02	7.13E+01
octanal	124-13-0	3.38E-01	1.50E+01	1.50E+01	6.00E+01	3.38E-01	8.14E+01	2.36E+00
o-dichlorobenzene	95-50-1	2.55E+01	3.75E+01	3.75E+01	1.50E+02	2.67E+01	2.16E+02	8.91E+00
o-methoxy-phenyl-azo-b-naphthol (oil red g)	1229-55-6	3.98E-01	3.75E+01	3.75E+01	1.50E+02	3.98E-01	4.14E+02	6.40E+00
o-xylene (ortho-xylene)	95-47-6	7.81E-01	1.50E+01	1.50E+01	6.00E+01	1.64E+00	1.44E+02	5.93E+00
particulate cyanide	57-12-5	3.57E+02	1.50E+01	1.50E+01	6.00E+01	3.57E+02	7.59E-01	3.95E+00
p-dichlorobenzene (para-dichlorobenzene)	106-46-7	3.34E+01	3.75E+01	3.75E+01	1.50E+02	2.67E+01	2.19E+02	8.91E+00
pentaerythritoltetranitrate (PETN)	78-11-5	6.59E+00	3.75E+01	3.75E+01	1.50E+02	6.59E+00	3.70E+01	9.92E+00
perchloroethylene	127-18-4	6.38E+01	6.00E+01	6.00E+01	2.40E+02	5.00E+01	2.09E+02	1.05E+01
phenanthrene	85-01-8	8.23E-01	6.00E+01	6.00E+01	2.40E+02	8.23E-01	3.83E+02	9.77E+00
phenol	108-95-2	4.07E-01	1.50E+01	1.50E+01	6.00E+01	3.20E-01	5.40E+00	4.30E+00
phenylacetylene (ethynyl benzene)	536-74-3	1.28E+00	1.50E+01	1.50E+01	6.00E+01	1.33E+00	5.02E+01	4.67E+00
phosphorus	7723-14-0	4.17E+03	1.50E+01	1.50E+01	6.00E+01	1.00E+06	7.55E-01	4.02E+00
propanal	123-38-6	5.46E-01	1.50E+01	1.50E+01	6.00E+01	4.86E-01	1.31E+00	3.09E+00
propane	74-98-6	9.30E+00	1.50E+01	1.50E+01	6.00E+01	8.43E+00	3.55E+01	4.11E+00
propylene	115-07-1	2.90E-01	1.50E+01	1.50E+01	6.00E+01	4.05E-01	1.02E+01	4.09E+00
propyne	74-99-7	1.81E+00	1.50E+01	1.50E+01	6.00E+01	1.50E+00	2.11E+00	4.07E+00

Table 24 (Concluded)

Chemical	CAS Number	Air[1]	Surface Water[1]	Soil[1]	Sediment[1]	Oxidation in Air	Biodegradation	
							Water	Soil
pyrene	129-00-0	2.14E-01	6.00E+01	6.00E+01	2.40E+02	2.14E-01	4.03E+02	1.85E+01
RDX	121-82-4	4.35E-02	3.75E+01	3.75E+01	1.50E+02	4.30E-02	1.89E+00	6.22E+00
selenium	7782-49-2	1.65E-01	1.50E+01	1.50E+01	6.00E+01	1.65E-01	9.54E-01	4.48E+00
silver	7440-22-4	4.17E+03	1.50E+01	1.50E+01	6.00E+01	1.00E+06	9.48E-01	4.77E+00
styrene (vinyl benzene)	100-42-5	1.37E-01	1.50E+01	1.50E+01	6.00E+01	3.80E-01	1.10E+02	4.69E+00
sulfur dioxide (SO2)	7446 09 5	1.78E-01	1.50E+01	1.50E+01	6.00E+01	1.78E-01	6.67E-01	4.31E+00
sulfuric acid	7664-93-9	3.82E+01	1.50E+01	1.50E+01	6.00E+01	3.82E+01	6.67E-01	4.66E+00
tetryl (2,4,6-trinitrophenylmethylnitramine)	479-45-8	8.45E+00	6.00E+01	6.00E+01	2.40E+02	8.45E+00	7.79E+00	1.22E+01
thallium	7440-28-0	4.17E+03	3.75E+01	3.75E+01	1.50E+02	1.00E+06	9.48E-01	5.97E+00
thiophene	110-02-1	1.12E+00	1.50E+01	1.50E+01	6.00E+01	1.12E+00	1.11E+01	4.51E+00
toluene	108-88-3	1.79E+00	1.50E+01	1.50E+01	6.00E+01	2.05E+00	7.41E+01	5.10E+00
trans-2-butenal	123-73-9	2.84E-01	1.50E+01	1.50E+01	6.00E+01	3.55E+00	1.33E+00	3.18E+00
trans-2-butene	624-64-6	5.77E-02	8.67E+00	8.67E+00	3.47E+01	2.27E+00	3.20E+01	2.74E+00
trans-2-pentene	646-04-8	2.96E-02	8.67E+00	8.67E+00	3.47E+01	2.23E+00	5.55E+01	2.83E+00
trans-3-penten-2-one	625-33-2	1.51E-01	1.50E+01	1.50E+01	6.00E+01	2.52E+00	1.22E+00	4.68E+00
trichloroethylene (TCE)	79-01-6	4.52E+00	3.75E+01	3.75E+01	1.50E+02	1.33E+01	4.02E+01	8.20E+00
trichloroflouromethane	75-69-4	4.17E+03	6.00E+01	6.00E+01	2.40E+02	1.00E+06	5.02E+01	1.07E+01
vinylidenechloride	75-35-4	9.81E-01	3.75E+01	3.75E+01	1.50E+02	4.72E+00	2.19E+01	6.43E+00
zinc	7440-66-6	4.17E+03	1.50E+01	1.50E+01	6.00E+01	1.00E+06	7.22E-01	4.34E+00

(Sheet 7 of 7)

Table 25
Model Comparison With Range Database Values

Estimation Software	N	Bias, days	AME, %
PBT air	118	-6.76E+02	2.56E+03
EPI air	120	-3.40E+02	5.21E+03
PBT soil	104	-1.52E+06	1.63E+03
EPI soil	105	-1.51E+06	7.96E+03
PBT water	115	-9.60E+01	4.14E+03
EPI water	118	-9.70E+01	1.01E+04

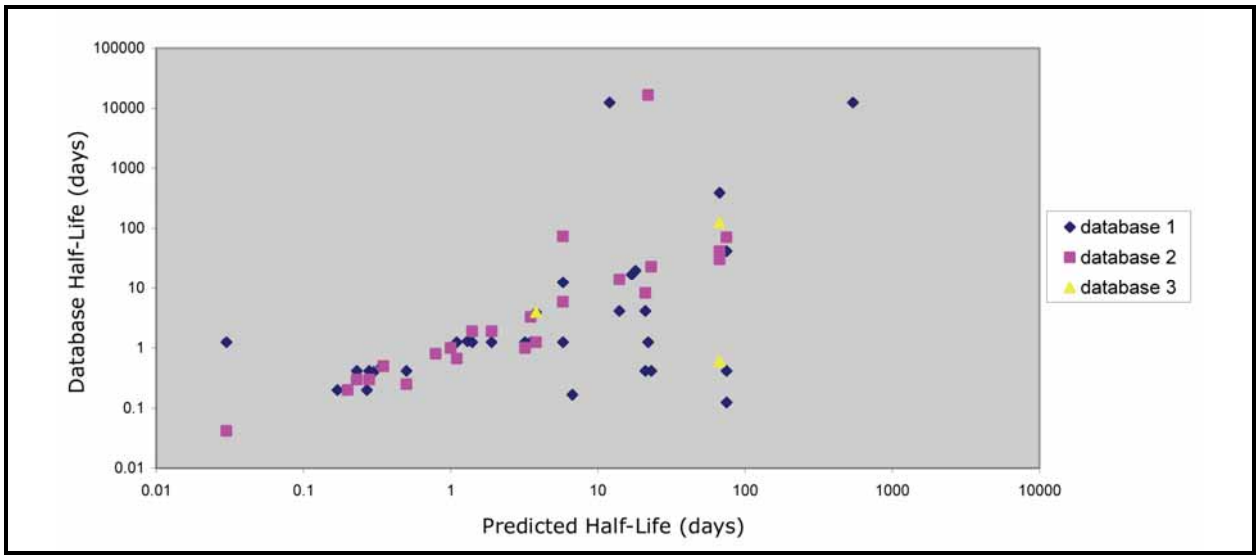


Figure 6. Comparison between Range Database version 1.5 air half-lives and half-lives predicted by PBT

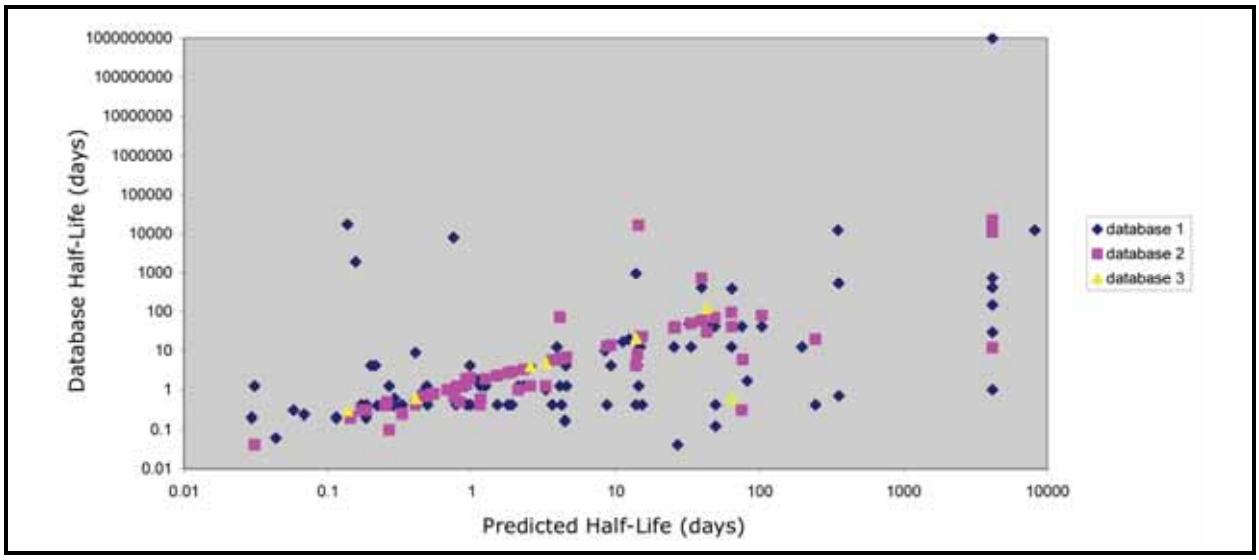


Figure 7. Comparison between Range Database version 1.5 air half-lives and half-lives predicted by EPI

result of recalcitrant compounds having measured half-lives of many years, but predicted half-lives of only a couple of months at most. Some recalcitrant compounds are found in most compound classes. The water AMEs were also thousands of percent, and although the negative biases were a comparatively small hundred days, the smaller bias for water in the presence of such huge model error merely reflects a more uniform data scatter than for soil, not a better model fit. The typical R^2 is much less than 0.1, so that R^2 is not an appropriate measure for this data set.

The large negative biases of a hundred or more days are the direct result of the limited time frames chosen for these model predictions, not the expert system queries nor the functional group formalism. These time frames were chosen to represent the most environmentally relevant time frames, but some recalcitrant compounds have much slower rates than can be captured by these models. The large negative biases could be eliminated by simply extending the time frames greatly, but the subsequent wider possible range for each compound is likely to lead to larger AME.

For soil and for water, the AMEs of thousands of percent are probably mostly due to the expert system approach. In this approach, rather than developing models representing measured data, the models represent consensus of a relatively small number of compounds in a small number of classes. It may be that the models represent that consensus with small model error, while having large model error in representing the measured data of a larger number of compounds in a larger number of compound classes.

In contrast, the AMEs of thousands of percent for air degradation rates are due to some fundamental failure of applicability of the assumptions used to derive the rates for the environmental conditions under which some of the rates were measured. One such fundamental assumption is that degradation in air is in the vapor phase, for instance, not on surfaces of particles, and not in droplets. Another assumption is that the vapor concentrations are small; another is that humidity is negligible. A minor limitation is that some of the kinetic oxidation parameter fits were originally made on a relatively small number of compounds in a limited class of compounds.

Comparisons and correlations, relative error, model error

The average bias (Equation 4) and percent AME (Equation 5) are the statistics used to compare predicted and observed results. For the purpose of this study, multiple observations for a compound will be treated as simply averaged among all observations, whereas each prediction will be considered as a point rather than a range. Thus, there is one bias and one AME for each EPI and PBT property. The bias and AME for each media half-life (air, soil, and water) are presented for PBT and EPI in Table 25. In the previously compiled values for the Range Database, an arbitrary large value of 1.0E+09 days had been entered for degradation rates for several compounds that had only open-ended “greater than” values reported at the time of compilation. These special large values were not included in the following analyses, although the large negative biases were

especially affected by other quite large database entries and corresponding small predictions.

R^2 and other fits for interpolation and extrapolation

There are other measures of model performance, especially the R^2 measure of goodness of fit, useful for interpolation and extrapolation of a small number of continuous parameters. Other kinds of measures are appropriate for non-continuous discrete classification type variables. These measures have a common feature of being applicable to observations and predictions that are represented as data points. When the spread of the data is important, or rather more generally when the data are not considered to be points but instead to be ranges of values, B-fitting using the Bhattacharyya measure (Thacker et al. 1996) is an alternative to least-squares fitting to develop a model of the data. In such cases, the data are not exact points but instead have error bars or general probability density distributions.

A least squares fit for data points will select the optimal model such that points on the model regression (typically, a linear fit) are closest to the data points. For instance, given the normal Euclidean metric, the closest points are where the line perpendicular to the model fit passes through the centroid of the data. Almost all common fitting algorithms implement versions of a least squares fit to develop models.

In B-fitting, the optimal model solution occurs when the data and model distributions have maximum overlap. The models obtained by least squares fitting and B-fitting may well be the same. But especially where the error bars or distributions are large or not isotropic, the B-fit model may differ significantly from the least squares fit.

Data Gaps

The degradation rates for all the chemicals in the main environmental matrices (air, soil, water) in the Range Database have all been filled by predictions from at least one software package. However, the data gaps for process-specific rates, especially hydrolysis and photolysis in water, still exist. In general, the degradation rates for a particular matrix or process are either all filled in (populated) for all compounds in the database or are all empty for all the compounds in the database due to the assumptions and limitations of the software. However, the filled in predicted values are quite uncertain due to the large biases and large AMEs identified by the analysis. Typically, the predicted half-lives are one to two orders of magnitude smaller than observed, although some of the observed values were also estimated. The primary cause of the error was identified as the limited range of predictions, whereas database values compiled from the literature had a wide range. Thus, although the original data gaps now have a better characterized uncertainty (i.e. a factor of one to two orders of magnitude as opposed to completely unknown), the current

predictions cannot be used to further the intended purpose of having an accurate reference tool for parameters of chemicals found on ranges.

The results of the analysis suggest improvements that could be made in the predictions. It was expected that rates of reaction in the environment would be too difficult to predict accurately for all compounds under all conditions. Of most immediate use would be modifications of the fits used to develop the current models to more accurately fit the data for air, soil, and water for the compounds in the Range Database. Separately, software packages could be developed that calculate rates of hydrolysis and photolysis of water.

The models used an expert system to rank degradation times as short, medium, or long, and used functional group contributions to predict the chemistry and rates of reaction. The same functional group formalism could be used not in the context of the expert system but in the context of trustworthy data already in the database. Such data already vary over a wide range, so that the primary error of limited predicted range is automatically addressed. Moreover, the best such fit will consequently have approximately zero bias. The development of the model could proceed along the minimization of model error, thereby minimizing the model error.

Thus, the problems of model bias (as applied to database values), model error, and model range are best addressed by using the database values in developing the model. The usual method of separating a fixed portion (e.g., a random one-fifth of each class) of the data for model testing instead of model development is recommended. The alternative leave-one-out round robin is easier to implement but more inclined to over-fitting.

Degradation rates are likely to remain highly uncertain. As noted previously, measuring degradation rates is costly and problematic because such rates are highly site- and chemical-specific. Field measurements and/or controlled laboratory experiments (with field-like conditions) should be coupled to more accurately determine rates. Additionally, future research in this area should include improving the predictive QSAR models. In the interim, conservative assumptions should be used in exposure assessment, i.e., long half-lives and high persistence in the environment.

7 Human Toxicological Benchmarks

Introduction

Initial screening efforts (Zakikhani et al. 2002) focused on data collection to determine if sufficient information was available to characterize risk. These efforts found considerable data gaps in substance-specific chemical/physical properties and toxicological values. The purpose of the present study was to rigorously investigate these gaps and determine: (1) if responsible surrogates exist, (2) if data exist that could be refined and used in the same manner, (3) if responsible chemical structural models exist to predict missing data, and (4) recommend specific research or testing to develop the data needed to derive values.

Specifically, this part of the present study focused on the development of chronic toxicity benchmarks for identified substances lacking such information. A hierarchy was followed to address these gaps. Initially, all substances were checked for the existence of chronic toxicity benchmarks (noncancer and cancer). If no benchmarks existed, then the literature was evaluated to determine if, at a minimum, any subchronic or chronic animal studies of sufficient quality were available. If so, these data were used to derive Reference Dose (RfD) and Reference Concentration (RfC) equivalent values. If sufficient subchronic or chronic data were not available, then chemical structure was available to derive an RfD surrogate using the Quantitative Structure Activity Relationship (QSAR) approach. When these relationships were weak, the recommended tests needed to develop the appropriate chronic benchmark were suggested.

Methods

The U.S. Army Environmental Center (AEC) provided the Center for Health Promotion and Preventive Medicine (CHPPM) a list of 188 tentatively identified compounds. For each chemical on this list, several databases were searched for the following applicable toxicity benchmarks:

- RfDs
- RfCs

- Cancer slope factors
- Minimum risk levels (MRLs)
- Maximum contaminant levels (MCLs)
- Provisional peer-reviewed toxicity values (PPRTVs)
- Chemical-specific cancer category and screening (e.g., in-vitro) information

It was identified that chronic general population benchmarks were needed to assess risk in a conservative scenario. This logic is based on the variation of potential applications for any given range (e.g., Base Realignment and Closure; Resource, Conservation and Recovery Act corrective actions; etc.) and that acute benchmarks usually precede the development of chronic ones (i.e., if there are subchronic toxicity data, there are often acute data from which to derive benchmarks also). These benchmarks are intended to apply to the general population and have been developed by the USEPA (1997b, 2001a, 2001b, 2004a). The methods for their derivation have been published and are well understood.

Cancer and noncancer risks are typically evaluated separately. Risk for noncancer effects is evaluated through the use of RfDs and RfCs for exposures from the oral and inhalation routes of exposure, respectively. Since many of these substances result in systemic effects in a chronic scenario, both are converted to an RfD equivalent (units of mg substance/kg body weight/day). RfCs were converted to an RfD_i (in mg/kg/day) by assuming a mean body weight of 70 kg and a mean daily air ventiltion volume of 20 m^3.

For many compounds, an RfD has not been established; however, subchronic toxicity data or a chronic benchmark may be available (e.g., Threshold Limit Value; TLV). For these substances, a provisional RfD equivalent has been developed, either from using identical methods as the USEPA or from time extrapolating from an occupational benchmark (i.e., TLV). These provisional benchmarks are not expected to be on a par with those developed from the USEPA from adequate chronic or subchronic toxicity studies according to prescribed criteria and review procedures. Rather, they are intended as screening tools, suited to situations where many pollutant compounds, widely varying in toxicity, coexist in a particular environment.

When suitable subchronic toxicity data or chronic occupational benchmarks do not exist, other provisional RfDs have been developed using a system of QSAR, which produces statistically based estimates of toxicological parameters (endpoints) in the absence of toxicity data on the compound in question. For this, the commercially available TOPKAT system (Accelrys, San Diego, CA) was used. This system is described more fully in Appendix A. In general, this system was used when experimental data were absent or inadequate or there was a lack of experimental data-based, noncancer benchmarks.

Cancer is the result of unregulated, often undifferentiated cell growth that has the potential to spread from one tissue to another. This is often the result of an alternation of genetic code (mutagenesis) or of promotion of cells that have corrupted genetic code. The propensity of cancer is determined through sound

human epidemiological data and/or controlled animal studies. Animal studies can be time and cost intensive;[1] hence, screening in-vitro methods have been developed to evaluate the likelihood of mutagenic events from chemical exposure. An evaluation of the cancer database for each substance by specific entities (e.g. USEPA) results in a determination for the likelihood of cancer in humans (Table 26).

Table 26
Cancer Classifications/Cancer Groupings Concordance

EPA Classification			IARC	ACGIH	NTP
< 1996	**1996-1999**	**1999 >**			
A Known human carcinogen	Known/likely	Human carcinogen	Group 1 Known carcinogen	A1 Confirmed human carcinogen	Known carcinogen
B1 Known animal carcinogen, human evidence limited		Likely human carcinogen	Group 2a Probable carcinogen	A2 Suspected human carcinogen	Reasonably anticipated to be carcinogen
B2 Sufficient animal evidence; inadequate human evidence					
C Possible human carcinogen (limited animal, no human data)	Cannot be determined	Suggestive evidence, insufficient to assess human carcinogenic potential	Group 2b Possible carcinogen	A3 Confirmed animal, unknown human relevance	
D Human carcinogenicity not classifiable (incomplete, inadequate, or ambiguous data)		Inadequate evidence to assess human carcinogenic potential	Group 3 Unclassifiable due incomplete or ambiguous data	A4 Not classifiable as human carcinogen	
E Probably not carcinogenic (no evidence from two tests in two animal species)	Not likely	Not likely to be human carcinogen	Group 4 Probably not carcinogen	A5 Not suspected as human carcinogen	

IARC = International Agency for Research on Cancer.
ACGIH = American Conference of Governmental Industrial Hygienists.
NTP = National Toxicology Program.

Estimation of provisional RfD from subchronic data or benchmark

The first step in development of the RfD was choice of a toxicity datum for calculation, based on a hierarchy of choice, with professional judgment being used in all cases:

a. An experimental chronic or subchronic NOAEL (no observed adverse effect level) or LOAEL (lowest observed adverse effect level).

[1] Newer methods integrate genetically altered laboratory rodents that are more cost and time efficient than earlier conventional 2-year exposure regimes.

b. A QSAR estimate of the rat chronic LOAEL, provided the reliability of the estimate was reasonably good.

c. An experimental NOAEL or LOAEL for a structurally related compound. In some cases this may take precedence over a QSAR estimate.

d. A QSAR estimate of the rat chronic LOAEL for a structurally related compound.

Where a TLV has been established for permissible exposure to the particular substance in the workplace, this value was sometimes used in calculation of the RfD. In such cases the RfD value derived from the TLV was compared to that derived from one or more of the other approaches.

Development of the RfD from a LOAEL or NOAEL requires the choice of an uncertainty factor (UF). UF will be in each case a matter of judgment, with an attempt to conform to USEPA guidelines (USEPA 1989). The LOAEL or NOAEL is divided by the UF to yield the RfD. The UF is the product of:

a. UFa - for interspecies variation, if datum is based on animal study, usually 10.

b. UFh -for intraspecies variation; accounts for sensitive human subgroups, usually 10.

c. UFs - for use of subchronic data (subchronic to chronic), usually 3 or 10.

d. UFl - for use of LOAEL (LOAEL to NOAEL), usually 3 or 10.

Additional UF that may be used are:

a. UFq - for use of a QSAR estimate, usually 3 or 10; considers reliability of estimate.

b. UFr - for use of structurally related compound, usually 3 or 10; depends on relatedness, including related function.

Other sources of uncertainty are covered by a modifying factor (MF), which must fall between 0.1 and 10 (default value = 1). The MF may reflect scientific uncertainties in a key study, or chemical-specific issues.

Any UF may be reduced, e.g., to 3 or 0, if justification exists. A total UF over 10,000 will not be used. The USEPA allows for some compression of the composite UF, recognizing that some dimensions of variability do not function independently, and that multiplying four or more factors of 10 is likely to yield an unrealistically conservative estimate of the RfD.

The resulting estimate of the RfD is provisional only and intended for screening and other limited purposes. Support from observational or experimental data is inadequate for RfD derivation and often absent altogether.

These numbers are presented as the best available and likely to be more realistic than can be gotten from alternative approaches, short of experimental data.

Estimation of provisional RfD using QSAR

For each QSAR estimate, an assessment is made as to its credibility (validity), and some uncertainty always remains unless the estimate is corroborated by good observational or experimental data. An extensive process of internal validation is automatically performed by the TOPKAT software for each estimate performed. Additional validation was performed by the user for each estimate. Further information on validation and validation procedures is presented in Appendix A.

Validation of each estimate includes, but is not limited to, the following:

a. The compound should fall within the multidimensional "Optimum Prediction Space" of the pertinent model.

b. The database present in the model should have all substructures of the query compound well represented.

c. The database should contain structures that are close to the query structure, and these should be predicted accurately by the model.

d. Database compounds that are close to the query compound should include some that are close to the query compound in toxicity.

Cancer evaluation

Risk from cancer is determined quantitatively through an evaluation of exposure to projected cancer incidence. The slope of the incidence is determined through an extrapolation of animal and/or human data and is known as a cancer slope factor (CSF). Databases were, therefore, searched to determine if there were published CSFs available. When CSFs were not available, substance-specific cancer classifications/grouping were reviewed to determine if regulatory jurisdictions determined if adequate evidence for cancer was available (e.g., not classifiable or determined as a carcinogen). If a cancer classification was not available, databases were searched for investigative screening procedures (i.e., in-vitro studies). Based on those data, a determination was made regarding any additional data requirements.

Results

Noncancer evaluation

Pertinent data and QSAR estimates are shown for each compound in Appendix B as well as in the following tables. Also shown are the estimates of Reference Dose and the approaches used to obtain them. A brief discussion of suggested estimates is also given in Appendix B for compounds in each structural group.

As shown in Appendix B Reference Dose values (RfD_o oral, RfD_i inhalation, or both) were found for 94 substances in the overall list of 188. For the remaining 94 substances, published RfDs were not found. For the compounds for which published RfDs were found, RfD estimates were unnecessary and, if made, were intended only for comparison purposes.

Of the 96 substances without published RfDs, provisional estimates of the RfD_o were made on most (68 substances). In 36 cases, the RfD estimate was derived solely from QSAR estimates, primarily of the estimated rat chronic LOAEL derived for each compound in question. These compounds are listed in Table 27.

Table 27
Compounds for Which Provisional RfD Estimate Was Based on QSAR Only

Compound	CAS Number	QSAR Est. of Rat Chronic LOAEL mg/kg/day	UF	Est. of RfD_o mgkg/day	Confidence in Est.	Recommendation
1,3-butadiene	106-99-0	201	3000	6.7 E-2	High	Acceptable as provisional RfD estimate
2-methyl-1-butene	563-46-2	414	3000	1.4 E-1	High	
benzo(e)pyrene	192-97-2	59	3000	1.2 E-1	High	
butanal	123-72-8	218	3000	7.3 E-2	High	
phenanthrene	85-01-8	119	3000	4.0 E-2	High	
1-methylamino anthraquinone	82-38-2	85.6	3000	2.9 E-2	Med.	
2,3-butanedione	431-03-8	18	3000	1.7 E-1	Med.	
2,5-dimethylfuran	625-86-5	6.9	3000	1.6 E-2	Med.	
2-methylfuran	534-22-5	20.8	3000	6.9 E-3	Med.	
2-methylthiophene	554-14-3	50	3000	1.7 E-2	Med.	
2-thiophene carboxaldehyde	98-03-3	54.8	3000	1.8 E-2	Med.	
3-(phenylhydrazone)-1H-indole-2,3-dione	17310-26-8	119	3000	4.0 E-2	Med.	
3-furaldehyde	498-60-2	11.5	3000	3.8 E-3	Med.	
3-methylthiophene	616-44-4	50	3000	1.7 E-2	Med.	
4-phenoxy-2(1H)-quinolinone (a)	66662-28-0	39	3000	1.3 E-2	Med.	
benzanthrone	82-05-3	178	3000	5.9 E-2	Med.	
benzo(a)anthracene	56-55-3	613	3000	2 E-1	Med.	
benzo(b)fluoranthene	205-99-2	370	3000	1.2 E-1	Med.	
benzo(k)fluroanthene	207-08-9	730	3000	2.4 E-1	Med.	

(Continued)

Table 27 (Concluded)

Compound	CAS Number	QSAR Est. of Rat Chronic LOAEL mg/kg/day	UF	Est. of RfD_o mgkg/day	Confidence in Est.	Recommendation
benzo(g,h,i)perylene	191-24-2	807	3000	4.2 E-2	Med.	Acceptable as provisional RfD estimate
benzonitrile	100-47-0	50.6	3000	1.7 E-2	Med.	
chrysene	218-01-9	308	3000	3.1 E-2	Med.	
cis-2-butene	590-18-1	338	3000	1.1 E-1	Med.	
heptanal	111-71-7	373	3000	1.2 E-1	Med.	
isobutene	115-11-7	480	3000	1.6 E-1	Med.	
nonanal	124-19-6	476	3000	1.6 E-1	Med.	
octanal	124-13-0	424	3000	1.4 E-1	Med.	
propanal	123-38-6	166	3000	5.5 E-2	Med.	
thiophene	110-02-1	45	3000	1.5 E-2	Med.	
trans-2-butenal	123-73-9	18.4[1]	3000	6.1 E-3	Med.	
trans-2-pentene	646-04-8	256	3000	8.5 E-2	Med.	
4-1,2,4-oxadiazolin-3-one-2,5-diphenyl delta	Not found	71	3000	2.4 E-2	Med.	
1,4-di-p-toluidino anthraquinone	128-80-3	166[1]	3000	5.5E-2	Low	Estimate of RfD less than acceptable; subchronic toxicity testing is needed
carbonyl sulfide	463-58-1	3.5[1]	3000	1.2E-3	Low	
indeno(1,2,3,cd) pyrene	193-39-5	131[1]	3000	4.4 E-2	Low	
isothiocyanato methane	556-61-6	11.5[1]	10,000	1.2 E-3	Low	
methylnitrite	624-91-9	1.3	10000	1.3 E-4	Low	
methoxy-phenylazo-b naphthol	1229-55-6	19[1]	3000	6.3E-3	Low	
phenylacetylene	536-74-3	52	3000	1.7E-2	Low	
trans-3-penten-2-one	3102-33-8	152[1]	3000	5.1E-2	Low	

[1] The lower 95 percent confidence bound of the rat chronic LOAEL estimate.
[2] The upper 95 percent confidence bound of the rat chronic LOAEL estimate.

Of the 40 provisional estimates of RfD_o in Table 27, all derived from QSAR information only, the assessment of confidence in the estimate is "high" or "medium" in the case of 32 compounds. For these, the indicated estimate of RfD_o is acceptable as a provisional answer, for limited purposes, pending further information. There remains the possibility that one or more of these compounds might be the subject of a published chronic or subchronic LOAEL or NOAEL that might serve as a basis for another estimate, based on experimental data. Such data have not been found.

For the remaining eight compounds the estimate was assessed as of "low" confidence. For these substances, any published chronic or subchronic, experimentally derived LOAEL or NOAEL has been sought for consideration as a possible basis for a provisional estimate of RfD. Such experimental findings have not been found, and the recommendation is that an appropriate subchronic or chronic study should be considered, depending on other factors, such as likelihood of human exposure.

A QSAR estimate of the rat chronic LOAEL was the basis for the sole provisional estimate of RfD_o in four additional cases (Table 28). But for these four chemicals, the QSAR estimate for a surrogate compound had to be used. A QSAR-based estimate on a surrogate compound also provided one of the estimates of RfD_o for pentaerythritol tetranitrate (PETN) (see Table 29).

Table 28
Compounds for Which Provisional Estimate of RfD_o Was Based Solely on QSAR Analysis on a Closely Related Surrogate Compound

Compound	CAS Number	Surrogate Compound	QSAR Est. Rat Chr. LOAEL mg/kg/day	UF	Est. of RfD_o mg/kg/day	Conf. in Est.	Recommendation
1,4-diamino-2,3-dihydro anthraquinone	81-63-0	1,4-diamino-anthraquinone	26.2	3000	8.7 E-3	Low	Estimate of RfD less than acceptable; subchronic toxicity testing is needed
3-methyl-1-butene	563-45-1	2-methyl-1-butene	414	10,000	4.1 E-2	Low	
3-methylfuran	930-27-8	2-methylfuran	20.8	10,000	2.1 E-3	Med	Acceptable as provisional RfD estimate
isobutane	75-28-5	n-butane	494	10,000	4.9 E-2	Med.	

Table 29
Compounds for Which Provisional RfD_o Estimates Were Made Both from QSAR Input and from Other Information, Arising from Experimental Or Observed Data

Compound	CAS Number	Basis for Estimate mg/kg/day or as stated	UF	Est. of RfD_o mg/kg/day	Conf. in Est. (QSAR)	Comment
1,2-dichloro-3-methylbenzene	32768-54-0	LOAEL, rat chr (QSAR) = 61 LOAEL, rat chr, rel cpd. o-Dichlorobenzene = 43	3000 1000	2.04 E-2 4.3 E-2	Med.	Two estimates similar
1-butene	106-98-9	LOAEL, rat chr (QSAR) = 204 RfD_o estimate for rel. cpd, 1-Hexene = 0.105	3000 3	3.5 E-2 3.5 E-2	Med.	Two estimates similar
1-chloro-3-methylbenzene	108-41-8	LOAEL, rat chr (QSAR) = 39 RfD_o, rel. cpd, 1-Chloro-2-methylbenzene (IRIS) = 2 E-2	3000 3	1.3 E-2 6.7 E-3	Med.	Two estimates similar
1-hexene	592-41-6	LOAEL, rat chr (QSAR) = 307 TLV (TWA; ACGIH) = 103 mg/m^3	3000 3	1.02 E-1 1.05 E-1	High	Two estimates similar
1-pentene	109-67-1	LOAEL, rat chr (QSAR) = 256 RfD_o estimate for rel cpd, 1-hexene = 0.105	3000 3	1.85E-2 3.5 E-2	Med.	Two estimates similar
2-heptanone	110-43-0	LOAEL, rat chr (QSAR) = 518 RfD_o, rel cpd 2-butanone = 6.0 E-1 (IRIS)	3000 3	1.7 E-1 2.0 E-1	High	Two estimates similar
2-pentanone	107-87-9	LOAEL, rat chr (QSAR) = 424 RfD_o, rel cpd, 2-Butanone = 6.0 E-1 (IRIS)	3000 3	1.4 E-1 2.0 E-1	High	Two estimates similar
2-propanol	67-63-0	LOAEL, rat chr (QSAR) = 174 TLV (TWA; ACGIH) = 980 mg/m^3	3000 100	5.8 E-2 1.0 E+0	Med.	Preferred est. = 5.8 E-2

(Continued)

Note that for one compound (PETN) the QSAR estimate is that for a related (surrogate) compound.

Table 29 (Concluded)

Compound	CAS Number	Basis for Estimate mg/kg/day or as stated	UF	Est. of RfD_o mg/kg/day	Conf. in Est. (QSAR)	Comment
4-amino-2,6-dinitrotoluene	19406-51-0	LOAEL, rat chr (QSAR) = 4.4 Publ. RfD_o for rel cpd. 2,4,6-TNT = 5 E-4 (IRIS)	3000 1	1.5E-3 5.0E-4	Med.	Two estimates similar
4-ethyltoluene	622-96-8	LOAEL, rat chr (QSAR) = 16.6 Publ. RfD_o for rel cpd, Ethylbenzene = 1.0 E-1 (IRIS)	3000 10	5.5 E-3 1.0 E-2	Med.	Two estimates similar
acenaphthalene	208-96-8	LOAEL, rat chr (QSAR) = 27.2 Publ. RfD_o for rel cpd, Acenaphthene = 6 E-2 (IRIS)	3000 3	9.1 E-3 2.0 E-2	High	Two estimates similar
acetic acid	64-19-7	LOAEL, rat chr (QSAR) = 120 TLV (TWA; ACGIH) = 24.5 mg/m^3	3000 100	4.0 E-2 2.5 E-2	Med.	Two estimates similar
ethanol	64-17-5	LOAEL, rat chr (QSAR) = 327 TLV (TWA; ACGIH) = 1900 mg/m^3	3000 100	1.1E-1 1.9E+0	Med.	Preferred est. = 1.9 E+0
hexanal	66-25-1	LOAEL, rat chr (QSAR) = 321 TLV (TWA; ACGIH) rel cpd, n-Pentanal = 175 mg/m^3	3000 100	1.1E-1 1.8E-1	High	Two estimates similar
methacrolein	78-85-3	LOAEL, rat chr (QSAR) = 22 Publ. RfD_o, rel cpd, Acrolein (IRIS) = 5 E-4	3000 1	7.3E-3 5.0 E-4	Med.	Preferred est. = 5 E-4
n-butane	106-97-8	LOAEL, rat chr (QSAR) = 494 Publ. RfD_o rel cpd, n-Hexane 6.0 E-2 (HEAST)	3000 1	1.6E-1 6.0E-2	High	Two estimates similar
methyl vinyl ketone	78-94-4	LOAEL, rat chr (QSAR) = 4.2 Publ. data; prov. LOAEL = 4.0	3000 3000	1.4E-3 1.3E-3	Low	Two estimates similar
n-decane	124-18-5	LOAEL, rat chr (QSAR) = 996 Publ. Rfd_o rel cpd, n-Hexane = 6.0 E-2 (HEAST)	3000 3	3.3E-1 2.0E-2	Med.	Preferred est. = 2.0 E-2
nitromethane	75-52-5	LOAEL, rat chr (QSAR) = 4.1 TLV (TWA; ACGIH) = 5.0 E+1 mg/m^3	3000 100	1.4E-3 5.0E-2	Med.	Preferred est. = 1.4 E-3
pentaerythritol tetranitrate (PETN)	78-11-5	LOAEL, rat chr (QSAR) for rel cpd 2,2-dimethyl-1,3-propanediol mono- Nitrate = 5.4 Clinical low dose (HSDB) – 0.43	3000 300	1.8E-3[1] 1.4E-3[1]	Low	Two estimates similar
propane	74-98-6	LOAEL, rat chr (QSAR) = 403 Publ. RfD_o rel cpd, n-Hexane = 6.0 E-2 (HEAST)	3000 1	1.3E-1 6.0E-2	Med.	Two estimates similar
propyne	74-99-7	LOAEL, rat chr (QSAR) = 103.5 TLV (TWA; ACGIH) = 1650 mg/m^3	3000 100	3.5E-2 1.7E+0	Low	Preferred est. = 1.7 E+0
2(2-quinolyl)-1,3-indandione	8003-22-3	LOAEL, rat chr (QSAR) = 10.1 Publ. data; prov. LOAEL = 120	3000 3000	3.4E-3 4.0E-2	Low	Preferred est. = 4.0 E-2

[1] A provisional RfD_o is not suggested here for PETN because the compound given to rodents in the feed is practically nontoxic.

For the first two compounds in Table 28, the estimate was assessed as of "low" confidence. For these substances, any published chronic or subchronic, experimentally derived LOAEL or NOAEL has been sought and considered as a possible basis for a provisional estimate of RfD. Such experimental findings

have not been found, and appropriate subchronic or chronic study should be considered, depending on other factors, such as likelihood of human exposure.

The final two compounds, 3-methylfuran and isobutane, are on somewhat better ground. For these the indicated estimate of RfD_o is acceptable as a provisional answer, for limited purposes, pending further information.

Five compounds on the list are the subject of provisional RfD_o estimates for which the basis of the estimate is derived solely from experimental/observational data. These are shown in Table 30.

Table 30
Compounds for Which Provisional RfD_o Was Estimated Solely from Experimental/ Observational Data

Compound	CAS Number	Basis for Estimate mg/kg/day or as stated	UF	Est. of RfD_o mg/kg/day	Recommendation
2-amino-9,10-anthracenedione	117-79-3	LOAEL, rat chr = 175	1000	1.8 E-1	Acceptable estimate
benzofuran	271-89-6	LOAEL, rat chr = 21.4	1000	2.1 E-2	Acceptable prov. estimate
nitroglycerin	55-63-0	Fed. Dr. Water Guideline = 5 µg/L; clinical dose 5 E-3	1 30	1.4 E-4 1.7 E-4	Est. based on human clinical dose is preferred
dichloroacetonitrile	3018-12-0	NOAEL, rat subchr = 8	1000	8.0 E-3	Acceptable estimate
dibenzo(b,def)-chrysene-7, 14-dione	128-66-5	LOAEL, rat chr = 350	1000	3.5 E-1	Acceptable estimate

The estimates of RfD_o for the above five compounds are acceptable as a provisional answer, pending further information. For nitroglycerin, the value preferred here is 1.7 E-4.

For many compounds lacking published RfDs, a provisional RfD_o was estimated from both QSAR input and other information, arising from experimental or observational data. Twenty-three compounds are in this category; these are listed in Table 29, along with RfD_o estimates and the basis for each estimate.

For 16 of the compounds in Table 29, the two RfD_o estimates, based on QSAR and on experimental/observational data, respectively, were quite close, within a factor of three or less. For these a recommendation would often be rather subjective, except for an overall suggestion that the lower of the two estimates be favored as the more conservative.

For the remaining seven compounds in Table 29, the two estimates are substantially different (factors of >3 to 50). In the case of methacrolein and n-decane, the estimate derived from the published RfD_o for a good surrogate compound is preferred here, i.e., 5 E-4 mg/kg/day for methacrolein and 2.0 E-2 mg/kg/day for n-decane. For 2-propanol, nitromethane, and propyne, there are two estimates, one based on QSAR and the other on TLV (TWA). The one based on QSAR is smaller in each case and includes a large UF, but may be preferable, due partly to the problems in reasoning from a short-term workplace

exposure to a chronic exposure that includes all population segments. In the case of ethanol and the yellow dye 2(2-quinolyl)-1,3-indandione, the higher estimate may be preferable, i.e., 1.9 E+0 for ethanol and 4.0 E-2 for the latter compound.

Of the 94 substances without previously published RfDs, there were 22 compounds for which the estimation of a provisional RfD value was not attempted. These are listed in Table 31, along with the reason for not attempting the estimate.

Table 31
Compounds Lacking Published RfD for Which Provisional RfD_o Estimates Are Not Provided

Compound	CAS Number	Reason for Not Developing Estimate	Comments
calcium	7440-70-2	Metal or inorganic	TOPKAT system for QSAR estimate is not designed to handle metals, organometals, or inorganic compounds
magnesium	7439-95-4		
lead	7439-92-1		
sulfur dioxide	7446-09-5		
sulfuric acid	64-67-5		
nitric acid	7697-37-2		
carbon monoxide	630-08-0		
carbon dioxide	124-38-9	Simple asphyxiants	No RfD estimate recommended. Hazard is from oxygen deprivation in confined spaces
methane	74-82-8		
ethane	74-84-0		
ethylene	74-85-1		
propylene (propene)	115-07-1		
acetylene	74-86-2		
benzo(a)pyrene	50-32-8	Hazard level is driven by cancer potency	Provisional RfD based on noncancer LOAEL or NOAEL not recommended
dibenz(a,h)anthracene	53-70-3		
2,3,7,8-tetrachlorodibenzo-p-dioxin	1746-01-6		
OCDD	3268-87-9		
(1,2-dichloroethyl) benzene	1074-11-9	QSAR estimate is unreliable	No basis found for an RfD estimate
dimethyl trisulfide	3658-80-8		
trans-2-butene	626-64-6	Cis-trans isomer of cis-2-butene	TOPKAT does not distinguish cis-trans configurations
1,2-dichloroethene (cis)	156-59-2	Cis-trans isomer of 1,2-dichloroethene (trans)	TOPKAT does not distinguish cis-trans configurations
xylene, mixed isomers	1330-20-7	Mixture	

Published RfD were not found for seven metals or inorganics. Provisional RfD estimates were not attempted on these because the TOPKAT system for QSAR does not encompass metals, inorganics, or organometallics.

The six small molecular weight gases shown in Table 31, carbon dioxide through acetylene, are classed as simple asphyxiants; i.e., the health hazard posed consists of oxygen deprivation at relatively high gas concentrations.

The two dioxins, TCDD and OCDD, have very high CSFs--out of proportion to the RfD--that would be derived with cancer not considered. Therefore, provisional RfDs are not suggested here. Among the several polycyclic aromatic hydrocarbons (PAHs) in the study, CSFs are very high for benzo(a)pyrene and

dibenz(a,h)anthracene. If a provisional RfD_o were suggested for any of these, with CSF not considered, the RfD would be very close to those suggested in this report for several closely related hydrocarbons, such as pyrene and benzo(b)fluoranthene. For strongly carcinogenic PAHs, the actual long-term safe level is much lower, 4 μg/L or below.

For (1,2-dichloroethyl) benzene and dimethyl trisulfide, the QSAR estimate was not reportable, and no suitable surrogate compound, or other basis for deriving a provisional RfD, was identified. For the dye substance 4-1,2,4-oxadiazolin-3-one-2,5-diphenyl-delta, no CAS number was found and it was felt that this leaves uncertainty about the identity of the exact substance referred to. Finally, an estimate was not attempted for trans-2-butene because an estimate has been provided for its cis isomer and TOPKAT does not distinguish between the two. The same applies to 1,2-dichloroethene (cis,) isomer of 1,2-dichloroethene (trans).

The RfD values of substances of concern for which published values or estimates were found at each step of the overall process are summarized in Figure 8. For example, of the 94 substances dealt with that lacked published RfD_o or RfD_i, provisional estimates were attempted on 72 substances. Of these, 28 compounds were found to have either experimental chronic or subchronic data or some chronic benchmark from which an estimate of RFD could be attempted. In most of these cases (23), QSAR estimates were simultaneously used and the resulting RfD estimates compared. In the case of 44 compounds, QSAR estimates alone were available. Of these 44, ten were identified as most likely to be in need of subchronic or chronic toxicity testing.

Cancer evaluation

CSFs are accepted estimates of human cancer risk. Substances having CSFs are not thought to require further carcinogenetic/mutagenic testing at this time. The 36 substances listed in Table 32, plus dioxin-TEQ, had reported CSFs.

Cancer classifications and groupings are a useful tool in roughly sorting substances according to generally accepted human carcinogenicity potential. Cancer classifications or cancer groups were found for 66 of the substances not having CSFs. These are listed in Tables 33 and 34, plus hexachlorocyclopentadiene (HCCPD).

HCCPD (CAS number 77-47-4), was designated Cancer Classification "E" (probably not carcinogenic) by the USEPA (2000) Integrated Risk Information System (IRIS). Therefore, additional mutagenicity/carcinogenicity testing is not recommended at this time.

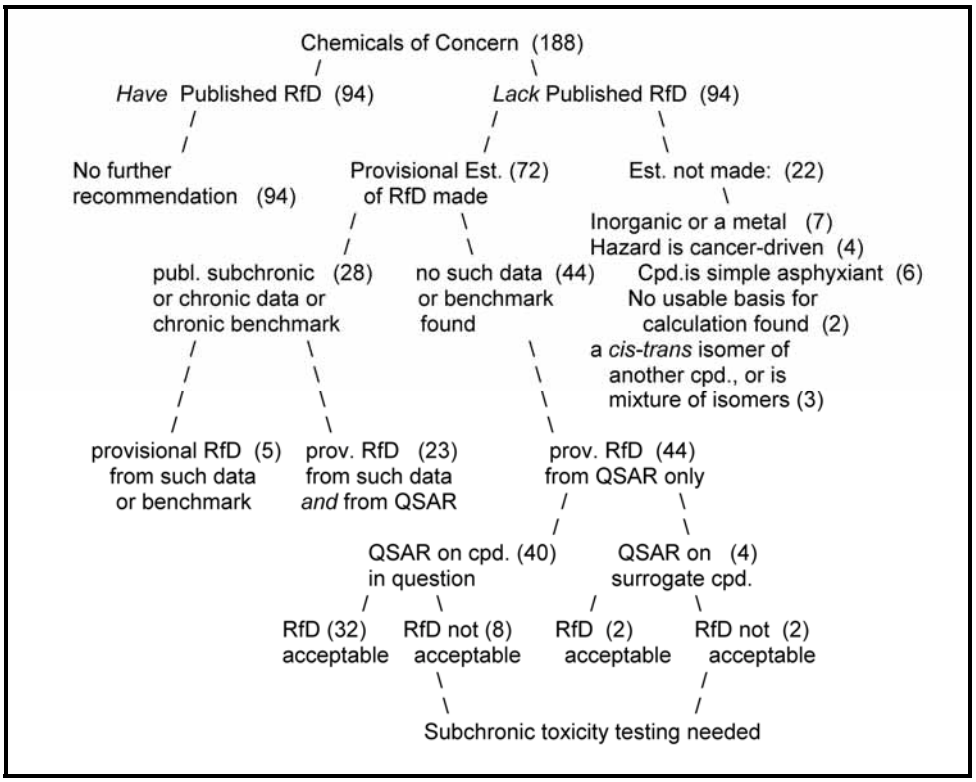


Figure 8. Decision tree for development of noncancer chronic benchmark RfDs

Table 32
Substances for Which CSFs Were Found. No Further Carcinogentic Testing Is Considered Necessary

Substance	CAS Number	Substance	CAS Number
1,2-dichlorethane	107-06-2	chloroform	67-66-3
2,3,7,8-tetracholorodibenzo-p-dioxin	1746-01-6	1,3-butadiene	106-99-0
2,4,6-trinitrotoluene	118-96-7	chloromethane (methyl chloride)	74-87-3
2-nitrotoluene (o-nitrotoluene)	88-72-2	chromium	7440-47-3
4-nitrotoluene (p-nitrotoluene)	99-99-0	chrysene	218-01-9
acetaldehyde	75-07-0	cobalt	7440-48-4
acrylonitrile	107-13-1	dibenz (a,h)anthracene (dba)	53-70-3
arsenic	7440-38-2	formaldehyde	50-00-0
benzene	71-43-2	hexachlorobenzene	118-74-1
benzo(a)anthracene	56-55-3	hexachlorobutadiene	87-68-3
benzo(a)pyrene	50-32-8	hexachloroethane	67-72-1
benzo(b)fluoranthene	205-99-2	methylene chloride	75-09-2
benzo(k)fluoranthene	207-08-9	ocdd (octachloradibenzo-p-dioxin)	3268-87-9
beryllium	7440-41-7	p-dichlorobenzene	106-46-7
bis(2-ethylhexyl)phthalate	117-81-7	perchloroethylene	127-18-4
cadmium	7440-43-9	RDX	121-82-4
carbontetrachloride	56-23-5	trans-2-butenal	123-73-9
chloroethene (vinyl chloride)	75-01-4	trichloroethylene	79-01-6

Table 33
Substances Likely to be Possible Human Carcinogens, Without CSFs

Substance	CAS Number	Further Testing
sulfuric acid	64-67-5	Yes, at micro-level carcinogenicity mode/mechanism
2,4-dinitrotoluene	121-14-2	Yes, animal studies from perspective of carcinogenicity mode/mechanism
2,6-dinitrotoluene	606-20-2	
lead	7439-92-1	
furan	110-00-9	
isothiocyanatomethane (methyl isothiocyanate)	556-61-6	
nitrobenzene	98-95-3	Yes. Insufficient animal or in-vitro evidence to support claimed B2 classification
nitromethane	75-52-5	
phenanthrene	85-01-8	Yes. Animal studies from perspective of carcinogenicity/ mutagenicity mode/mechanism, on specific substance, rather than substance as part of mixture or compound, or by surrogate substance of same type or similar structure
nickel	7440-02-0	
indeno(1,2,3-cd)pyrene	193-39-5	
benzofuran	271-89-6	Yes. Although sufficient evidence of carcinogenicity in animals, studies are needed to update, fill gaps, and resolve questions in National Toxicological Program (NTP) (1990) study
chlorobenzene	108-90-7	
2-furaldehyde (furfural)	98-01-1	
ethylchloride	75-00-3	Yes. Currently insufficient and/or contradictory experimental animal and in-vitro evidence of carcinogenicity and mutagenicity
methyl-t-butylether (MTBE)	1634-04-4	
styrene	100-42-5	
1,1-dichloroethylene (1,1-DCE) (vinylidenechloride)	75-35-4	

Table 34
Substances With "Unclassified" Cancer Potential

Substance	CAS Number	Comments
acenaphthylene	208-96-8	In-vitro testing may be advisable. Probable teratogen. Further animal testing may be indicated
HMX	2691-41-0	In-vitro testing may be advisable
phosphorus (white phosphorus)	7723-14-0	In-vitro testing may be advisable
HCl (hydrogen chloride)	7647-01-0	Further in-vitro testing may be advisable. Teratogen and mutagen (presumptive)
dichloroacetonitrile	3018-12-0	No further in-vitro required testing at this time, but may be advisable. Probable teratogen
particulate cyanide	57-12-5	No further in-vitro testing required at this time, but might be advisable
silver	7440-22-4	No further in-vitro testing required at this time
sulfur dioxide (SO2)	7446-09-5	No further in-vitro testing required at this time, but might be advisable
1,3-dinitrobenzene	99-65-0	No further in-vitro testing required at this time. Animal testing indicated
1-butanol (n-butanol)	71-36-3	No further in-vitro testing required at this time. Animal testing indicated
2-amino-9,10-anthracenedione (a)	117-79-3	No further in-vitro testing required at this time, but might be prudent given no apparent follow-up to NTP's 1983 "Reasonably anticipated to be a human carcinogen"
2-butanone (methyl ethyl ketone (MEK))	78-93-3	No further in-vitro testing required at this time.
2-propanol (isopropanol)	67-63-0	No further in-vitro testing required at this time. Generally Recognized as Safe (GRAS) list substance
3-nitrotoluene (m-nitrotoluene)	99-08-1	No further in-vitro testing required at this time
4-methyl-2-pentanone (methyly isobutyl ketone) (MIBK)	108-10-1	No further in-vitro testing required at this time
acetone	67-64-1	No further in-vitro testing required at this time
acetonitrile	75-05-8	No further in-vitro testing required at this time

(Continued)

Table 34 (Concluded)

Substance	CAS Number	Comments
acetophenone	98-86-2	No further in-vitro testing required at this time
acrolein, (2-propenal)	107-02-8	No further in-vitro testing required at this time
anthracene	120-12-7	No further in-vitro testing required at this time
barium	7440-39-3	No further in-vitro testing required at this time
benzo(e)pyrene	192-97-2	No further in-vitro testing required at this time
benzo(g,h,i)perylene	191-24-2	No further in-vitro testing required at this time
Cl2 (a) (chlorine)	7782-50-5	No further in-vitro testing required at this time
copper	7440-50-8	No further in-vitro testing required at this time
dibenzo(b,def)chrysene-7,14 dione (c. i. vat yellow 4)	128-66-5	No further in-vitro testing required at this time
dibutyl phthalate	84-74-2	No further in-vitro testing required at this time
diphenylamine	122-39-4	No further in-vitro testing required at this time
ethanol	64-17-5	No further in-vitro testing required at this time
ethylene	74-85-1	No further in-vitro testing required at this time
ethyl benzene	100-41-4	No further in-vitro or animal testing required at this time; inadequate animal model exists
fluoranthene	206-44-0	No further in-vitro testing required at this time
fluorene	86-73-7	No further in-vitro testing required at this time
manganese	7439-96-5	No further in-vitro testing required at this time
m-dichlorobenzene	541-73-1	No further in-vitro testing required at this time
mercury	7439-97-6	No further in-vitro testing required at this time
methane	74-82-8	No further in-vitro testing required at this time. Simple asphyxiate
nitrogen oxide (NOx)	10024-97-2	No further in-vitro testing required at this time
o-dichlorobenzene	95-50-1	No further in-vitro testing required at this time
o-xylene	95-47-6	No further in-vitro testing required at this time
phenol	108-95-2	No further in-vitro testing required at this time
propylene (propene)	115-07-1	No further in-vitro testing required at this time. Simple asphyxiate
p-xylene	106-42-3	No further in-vitro testing required at this time
pyrene	129-00-0	No further in-vitro testing required at this time
selenium	7782-49-2	No further in-vitro testing required at this time
toluene	108-88-3	No further in-vitro testing required at this time
zinc	7440-66-6	No further in-vitro testing required at this time

The 18 substances having possible, suspected, reasonably anticipated, probable, or confirmed carcinogen designations are listed in Table 33, together with specific testing recommendations.

Forty-seven substances having a carcinogenic potential designated by USEPA, IARC, or ACGIH as "unclassifiable," or equivalent, are listed in Table 34, together with specific considerations for further testing. Overall, these substances--for which there is insufficient or conflicting data, no positive evidence, no data solely relative to humans, or it is/was unsuitable for testing using (then) currently available methods--are considered to have a low priority for further testing.

Mutagenicity in-vitro can be a strong indicator of potential carcinogenicity in-vivo; therefore, in-vitro studies can be useful both in identifying mutagenicity and screening for potential carcinogenicity. Eighty-four substances had neither cancer classification, cancer group, nor other designation of potential carcinogenicity.

Table 35
Candidate Substances for In-Vitro Cancer Screening

Substance	CAS Number	Carcinogenicity/Mutagenicity In-Vitro Analysis Recommendation
(1,2-dichloroethyl)-benzene (styrene dichloride) (phenyldichloroethane)	1074-11-9	None. Insufficient information located to determine suitability for traditional in-vitro carcinogenicity analysis
1,2-dichloro-3-methylbenzene	32768-54-0	
i-butene/isobutylene	115-11-7	
1-hexene	592-41-6	
1-methylaminoanthraquinone (quinolin yellow)	82-38-2	
1-pentene	109-67-1	
2-methyl-1-butene	563-46-2	
2-thiophenecarboxaldehyde	98-03-3	
3-(phenylhydrazone)-1H-indole-2,3-dione	17310-26-8	
3-furaldehyde (3-furancarboxaldehyde)	498-60-2	
3-methyl-1-butene	563-45-1	
carbonyl sulfide	463-58-1	
phenylacetylene	536-74-3	
trans-3-penten-2-one	3102-33-8	
4-phenoxy-2(1H)-quinolinone (a)	6666-28-0	
1-butene	106-98-9	None. Simple asphyxiants unsuited to traditional in-vitro analysis
acetylene	74-86-2	
carbon dioxide (CO2)	124-38-9	
cis-2-butene	590-18-1	
ethane	74-84-0	
propane	74-98-6	
trans-2-butene	624-64-6	
trans-2-pentene	646-04-8	
3-methylfuran	930-27-8	Not recommended, biological VOC
antimony	7440-36-0	None. Elements unsuited to traditional in-vitro analysis
calcium (elemental)	7440-70-2	
magnesium	7439-95-4	
thallium	7440-28-0	
carbon monoxide (CO)	630-08-0	None. Probably unsuited to traditional in-vitro analysis
hydrogen cyanide	74-90-8	
2-pentanone (methyl propyl ketone)	107-87-9	None at this time. Food, food additive, flavor, scent, and drug additive components and/or by-products within FDA oversight
dimethyltrisulfide	3658-80-8	
methylnitrite	624-91-9	
octanal (octylaldehyde)	124-13-0	
i-butane (isobutane)	75-28-5	In-vitro carcinogenicity tests plausible, but not recommended

Out of 84 substances without carcinogenicity designation, no in-vitro information was located for the 35 substances listed in Table 35. Publication of in-vitro studies was often not available (or likely necessary) for substances such as food components and additives and supplements, flavors, scents, and cosmetics, "generally recognized as safe (GRAS)," or naturally occurring substances involved in U.S. Food and Drug Administration (FDA), patent, trademark, or proprietary issues. Most of the published research is at least 25 years old and does not necessarily reflect current scientific knowledge--such as subcellular mechanisms, DNA sequences, or cross-species applicability. Subject to individual chemical and physical properties, and both in-vitro and human biological principles, these 35 substances may or may not be candidates for in-vitro cancer screening.

In-vitro mutagenicity information was located for the 49 substances without designated carcinogenicity potential listed in Table 36. Three of these were reported as positive for in-vitro mutagenicity and should be evaluated for appropriate further studies, and 19 reportedly demonstrated both positive and negative mutagenicity and require further investigation. No further in-vitro testing is recommended at this time for the 27 substances reported as having only negative in-vitro test results.

Table 36
Substances with In-Vitro Mutagenicity Information

Substance	CAS Number	Recommendations
1,3,5-trinitrobenzene	99-35-4	Positive in-vitro data, negative animal data; no testing recommended
2,3-butanedione (diacetyl)	431-03-8	Positive mutagenicity in-vitro.
tetryl	479-45-8	Chronic cancer studies in experiment animals, and/or mechanistic level studies, may be warranted
1,4-diamino-2,3-dihydroanthraquinone	81-63-0	Both positive and negative mutagenicity in-vitro
1,4-di-p-toluidinoanthraquinone (quinzarine green; solvent green 3)	128-80-3	
2-(2-quinolyl)-1,3-indandione (solvent yellow 33, yellow no. 11 D&C)	8003-22-3	
2-amino-4,6-dinitrotoluene	35572-78-2	
4-amino-2,6-dinitrotoluene	19406-51-0	
benzaldehyde	100-52-7	
benzanthrone (b)	82-05-3	
butanal	123-72-8	
hexanal (hexaldehyde)	66-25-1	
methacrolein	78-85-3	
methyl-vinyl ketone	78-94-4	
naphthalene	91-20-3	
nitroglycerine	55-63-0	
nonanal (n-nonyl aldehyde)	124-19-6	
o-methoxy-phenyl-azo-b-naphthol (oil pink, c,.i.solvent red 1)	1229-55-6	
propanal	123-38-6	
propyne	74-99-7	
dichlorodiflouromethane (freon 12)	75-71-8	Mutagenicity negative in pre-1980 plant (*Tradescantia specia*) and positive in fungal (*Neurospora crassa*) in-vitro systems. Bacterial and mammalian in-vitro mutagenicity tests, at mechanism of action level, might be advisable
2-(2-quinolyl)-(h-indene-1,3-(2h)-dione (a); (1h-indene-1,3(2h)-dione,2-(2-quinolyl)-); (quinophthalone); (pigment yellow 138); (quinoline yellow)	83-08-9	Original literature review and/or of FDA or proprietary information needed. Apparently mixed response in one abstract located.
2-heptanone	110-43-0	Undetermined. Further studies may or may not be advisable. Two negative 2001 studies.
aluminum	7429-90-5	Undetermined. Further studies may or may not be advisable. Unavailable negative study or studies reported.
nitric acid	7697-37-2	Further studies are probably indicated. One negative pre-1980 study.

(Continued)

Table 36 (Concluded)

Substance	CAS Number	Recommendations
1,2,4-trimethylbenzene	95-63-6	Negative in-vitro studies. Further in-vitro testing not indicated at this time
1,2-dichloroethene	540-59-0 cis	
1,2-dichloroethene	540-59-0 trans	
1,3,5-trimethylbenzene	108-67-8	
1-chloro-2-methylbenzene	95-49-8	
1-chloro-3-methylbenzene (m-chlorotoluene)	108-41-8	
2,5-dimethylfuran	625-86-5	
2-methylfuran	534-22-5	
2-methylthiophene	554-14-3	
3-methylthiophene	616-44-4	
4-ethyltoluene	622-96-8	
acenaphthene	83-32-9	
acetic acid	64-19-7	
benzonitrile	100-47-0	
carbon disulfide	75-15-0	
heptanal	111-71-7	
n-butane	106-97-8	
n-decane	124-18-5	
NH3 (ammonia)	7664-41-7	Negative in-vitro studies. Further in-vitro testing not indicated at this time
n-hexane (hexane)	110-54-3	
m-xylene	108-38-3	
pentaerythritoltetranitrate (PETN)	78-11-5	
thiophene	110-02-1	
trichloroflouromethane	75-69-4	

Discussion

Uncertainty

Toxicity information is sparse for many of these compounds. This is due in part to the effort and ethical constraints required to conduct animal studies to provide meaningful results. These data are used by professionals to derive values intended to represent safe exposure levels. Considering the variability and conditions of dose-response data from these types of studies, human exposure/effect information, and other pertinent data, toxicologists and health professionals derive these values. Promulgated values from regulatory agencies and others (e.g. American Industrial Health Association, American Conference of Governmental Industrial Hygienists, etc.) are most rigorous since the data are used in a weight-of-evidence approach and values determined based on consensus. Although these values were sought, they were only available for roughly half of these identified compounds. Often this is due to a lack of pertinent toxicity information.

Since promulgated values were not available for many compounds, other methods were used. The use of the QSAR approach evaluates similarities in

chemical and toxicological attributes between substances and uses that information to estimate a toxicity endpoint (e.g., chronic rat LOAEL). That estimate is then converted into an RfD-like value using generally accepted techniques. This process provides the investigator with a confidence estimate that is based on structural similarities between compounds and their effect. However, such values are not fail-safe and are not equivalent to promulgated RfD values. Differences in toxicity may be pronounced between very similar compounds; hence these values are intended to be used only to make provisional risk estimates when the collection of relevant toxicity information is not feasible. Consequently, these QSAR-derived values are only more useful than no information at all and should be used with caution.

Caveats

Although regulatory promulgated values have the highest confidence level in this report, they are not without data insufficiencies. Uncertainty factors may be reduced on the basis of specific toxicological research, resulting in more realistic risk predictions and significant reductions in cleanup costs. Specific examples include ongoing work on RDX and perchlorate. These efforts, conducted in coordination with regulatory agencies, have been productive in providing more accurate information regarding toxicity. Through research using the latest methods, animal to human extrapolation of data can be enhanced and uncertainty reduced.

Concordances between cancer classifications and groupings--determined by different organizations, based upon different criteria or from different perspectives, or based on research by the same organization at different times--must be considered tentative. For example, “unclassifiable” and “cannot be determined” may mean insufficient or conflicting data, no positive evidence, solely related to human carcinogenicity, or substance cannot be tested using currently available methods. The National Toxicology Program (NTP) (1990), on the other hand, limits groupings to known and anticipated carcinogens. The USEPA has had three cancer classification systems, based upon different criteria and/or data interpretations, since 1986. The International Agency for Research on Cancer (IARC), a part of The World Health Organization (WHO), uses a system similar to the one USEPA abandoned in 1996, but with different underlying criteria, as does the American Conference of Governmental Industrial Hygienists (ACGIH), whose perspective is more concerned with cancer potentials resulting from occupational exposures.

Recommendations

The approach used in this study evaluated the prevalence of appropriate toxicity information in a logical format. However, this research was conducted lacking exposure information. Therefore, the recommendations made in this report are based on the prevalence of toxicity data only. To provide a proper risk-based approach, these substances should be evaluated based on exposure estimates. This process should also consider the appropriate human exposure

groups (e.g., soldiers, workers, residents, children, pregnant females, etc.), persistence and mobility in the environmental media, and consideration of the most likely exposure route (e.g., inhalation, oral, dermal). The amount of these substances found at the exposure point (concentration terms) should also be ascertained. Through this type of an evaluation, compounds most in need of data could be ranked and prioritized.

It is recommended that, at a minimum, subchronic in-vivo (rodent) toxicity testing is needed for compounds for which RfDs or RfD-equivalent values could not be developed. A minimum dataset from which to derive a RfD value requires a 90-day subchronic toxicity test. These tests are inclusive of an acute and subacute evaluation (i.e., a single and a 14-day repetitive-day exposure regime). These tests are expensive and require significant effort. They should also be conducted according to the highest standards of laboratory conduct (e.g., Good Laboratory Practices, 40 CFR Part 160) to provide relevant and accurate data acceptable to reviewers and regulatory authorities. The priority of such studies, however, should be based on the magnitude of exposure and best professional judgment.

Summary and Data Gaps

Of the 188 chemicals of concern, 94 have published Reference Doses (oral, inhalation, or both). For the remaining 94 substances, published information was sought from which to derive a provisional RfD. Such information would be either data on subchronic or chronic toxicity or a chronic toxicity benchmark such as the TLV.

If such information was not found, derivation of a provisional RfD was attempted using QSAR. In many cases an estimated provisional RfD was developed from both QSAR and experimental data.

For most of the 94 substances on the list without published RfDs, an effort was made to develop a preliminary, provisional estimate of the RfD_o, for screening or other limited purposes. Exceptions (listed in Table 31) included:

- Metals, inorganics - seven substances.
- Simple asphyxiants – six substances.
- Any substance for which a reasonably credible estimate, even at low confidence, could not be made from information at hand.
- Any substance that is known to have a high cancer potency (high CSF).

Estimates of RfD were made from published data, LOAEL or NOAEL, standards or benchmarks, and estimates of toxicity. For most compounds, QSAR values were estimated, either as the sole estimate or for comparison.

In many cases, information on a closely related (surrogate) compound was used. This might be either published information or a QSAR estimate. The frequency with which each method was used is as follows. Because these categories are not mutually exclusive, the numbers do not add up to total compounds estimated.

Category	No. of Compounds
A published RfD for a closely related compound	10
A published NOAEL or LOAEL	4
A published NOAEL or LOAEL for a related compound	1
The published TLV (TWA) (ACGIH)	6
Published TLV for a related compound	1
A Federal or State Drinking Water Guideline	1
A lowest dose in clinical practice (estimate of LOAEL)	2
A QSAR estimate of the rat chronic LOAEL	32
QSAR est. of rat chronic LOAEL for a related compound	2
QSAR est. of rat chronic LOAEL and a second est. based on experimental data	21

For 44 compounds, the RfD_o was estimated solely from QSAR data, including four cases in which the QSAR estimate was that for a related, or surrogate, compound. For most of the remainder, 23 compounds, both QSAR-based and other estimates were available for comparison.

The compounds having estimates of provisional RfD that were based on QSAR estimates where the confidence in the estimate is of low reliability are shown below and also in Appendix B. It is recommended that these be considered for possible subchronic toxicity testing, after consideration of other factors such as human exposure potential:

Compound	CAS Number
1,4-Di-p-toluidino anthraquinone	(128-80-3)
Isothiocyanato methane	(556-61-6)
o-Methoxy-phenylazo-b-naphthol	(1229-55-6)
Carbonyl sulfide	(463-58-1)
Indeno(1,2,3,cd) pyrene	(193-39-5)
Phenylacetylene	(536-74-3)
trans-3-Penten-2-one	(3102-33-8)
Methylnitrite	(624-91-9)
1,4-Diamino-2,3-dihydroanthraquinone	(81-63-0)
3-Methyl-1-butene	(563-45-1)

The basis of the RfD estimates, together with both QSAR information and other data, are summarized elsewhere, where the various structural groups of organic substances, e.g., alkanes, ketones, PAHs, etc., are dealt with separately.

8 Database Structure

The Range Database that was developed during the initial effort (Zakikhani et al. 2002) (http://el.erdc.usace.army.mil/arams/dbform.html) lists values for 11 physicochemical properties from five data sources and 14 toxicological benchmarks from data searches. As a result of the present study, the Range Database is being greatly expanded to include many additional parameters for human exposure and fate/transport from a host of data sources/methods. The new database must have a new interface for viewing more diverse data sources, number of parameters, and number of values for each of the parameters. Therefore, there was a need to totally redesign the database structure to accommodate the expansion.

The new design is relational in structure and organizes the data into seven tables (Constituents, Parameters, Range Values, Reference, Data Source, Data Type, and Synonyms) as discussed below.

The Constituents table lists the CAS ID, primary name, and class for each of the chemicals in the Range Database. The table contains fields as shown and described in Table 37.

Table 37
Constituents Table

FieldName	Data Type	Description
CasNo	Text	The Chemical Abstract Service Registry Number of the constituent (e.g., 118-96-7)
ConstituentName	Text	Name of the constituent
ConstituentClass	Text	Chemical class of the constituent (e.g., radionuclide, PAH, carboxylic acid, etc.)

The Parameters table is intended as the master list of parameters that could be stored in the database. Ideally, the Parameters table should contain parameters/ properties such as dermal absorption fraction, molecular weight, bioaccumulation factors, etc., and not any superfluous information, although the structure of the database does allow for this should the need arise. This table lists each of the parameters being examined in this study, assigns a unique ID number to each one, provides a description of the parameter, and allows the highest and lowest possible values for the parameter to be assigned as well as the units for the

parameter. Additionally, comments on the parameter can be made. The table contains the fields shown and described in Table 38.

Table 38
Parameters Table

FieldName	Data Type	Description
ParameterID	Integer	A unique numeric ID for the parameter (e.g., for K_{ow} the ParameterID may be 1)
ParameterName	Text	Name of the parameter (e.g., K_{ow}, K_{oc}, HLC, etc.)
ParameterDescription	Text	Description of the parameter (e.g., octanol-water partition coefficient, carbon matter partition coefficient)
LowRangeValue	Text	The lowest expected value for the parameter (e.g., the lowest expected value for Henry's law constant is 0)
HighRangeValue	Text	The highest expected value for the parameter (e.g., the highest expected value for Henry's law constant is 100 or perhaps even lower)
ParameterRangeUnits	Text	The units associated with the specified low and high values
Comments	Text	Any comments about the parameter may be added in this field

In this project, most of the calculated values were statistically analyzed in the same manner in an effort to provide an estimate of how good the calculated values actually are. Therefore, calculated parameters (e.g., diffusion coefficient in water, Dw) can have an associated absolute mean error (e.g., "Dw_AME") and average bias (e.g., "Dw_AvgBias"). This information is not stored in the database because it is planned for incorporation into the database browser interface that will be developed later for the database. Incorporating error statistics into the database browser interface allows for dynamic, up-to-date statistics as new data are added, which should be more beneficial to the user and make database maintenance easier. The database design encompasses the use of both calculated parameter values and measured parameter values. The "statistics" provided by the database browser interface would apply only for calculated parameter values.

The RangeValues table consists of fields to store information related to parameter values for the Range Database. This table lists the CAS ID of a chemical in the study, a parameter ID number from the Parameters table, the value for the parameter, the units of the value, the reference ID from which the value was obtained, the data source ID from which the value was obtained, the data type ID for the value, and a comment field to provide any comments that the user feels necessary for clarifying the specified value. The table contains the fields shown and described in Table 39.

The Reference table consists of fields to store information related to references for a data value. Typically, a reference is used to specify where a given parameter/property value can be found in a book, document, etc. A reference is generally more specific than a data source, which is described in the following section. The Reference table lists a short and full description for each of the references reported and assigns a unique ID number to each. The table contains the fields shown and described in Table 40.

Table 39
RangeValues Table

FieldName	Data Type	Description
CasNo	Text	The constituent Chemical Abstract Service Registry Number for which the parameter applies
ParameterID	Integer	The parameter ID
Value	Text	The value for the parameter
Units	Text	The units for the parameter value (e.g., K_{ow} may have units of mL/mL or mL/g)
ReferenceID	Long integer	An identifier for the associated reference from which the parameter value was obtained
DataSourceID	Integer	An identifier for the information source from which the parameter values were obtained
DataTypeID	Integer	An identifier to indicate the data type of the parameter value
Comments	Text	Any comments about the value may be specified in this field

Table 40
Reference Table

FieldName	Data Type	Description
ReferenceID	Long Integer	A unique numeric ID for the reference
ShortReference	Text	A short name for the reference (e.g., USEPA 1996, Soil Screening Guidance: Technical Background Document. EPA/540/R95/128. Office of Emergency and Remedial Response, Washington, DC. NTIS PB96-963502. may have a short reference of "USEPA (1996)")
FullReference	Memo	The full reference citation (e.g., USEPA 1996, Soil Screening Guidance: Technical Background Document. EPA/540/R95/128. Office of Emergency and Remedial Response, Washington, DC. NTIS PB96-963502.)

The DataSource table consists of fields to store information related to the source of the data. Data sources are typically databases, web sites, or books that may contain various different estimation equations and their references. Data sources are generally more generic than references. An estimation equation and its literature reference should be addressed in the Reference table, and the book that presents the equation along with other estimation equations should be addressed in the DataSource table. This table lists a short and full description for each of the data sources used and assigns a unique ID number to each. The table contains the fields shown and described in Table 41.

Table 41
DataSource Table

FieldName	Data Type	Description
DataSourceID	Integer	A unique numeric ID for the source of data
DataSourceShort	Text	A short name for the data source (e.g., "RAIS Database," "EPI Suite software," a book name, etc.)
DataSourceFull	Text	The full name of the data source

The DataType table consists of fields to store information related to the type of data. The available data types are experimental/measured (EXP), extrapolated (EXT), estimated (EST), calculated (CALC), and reported in literature, but

method of determination unknown, i.e., not available (N/A). These five data types are standards, but other data types can be added as necessary. The EST and CALC data types are similar and either may be appropriate for some data. The table contains the fields shown and described in Table 42.

Table 42
DataType Table

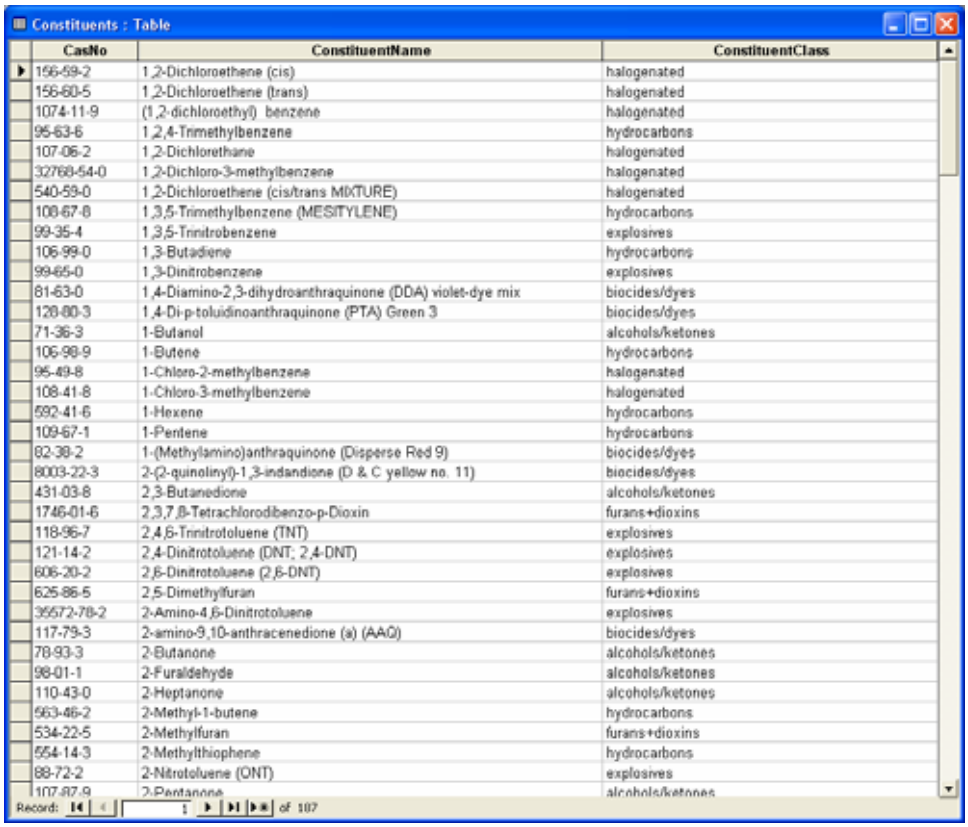
FieldName	Data Type	Description
DataTypeID	Integer	A unique numeric ID for the data type
DataType	Text	The name of the data type (e.g., these may include: experimental/measured (EXP), extrapolated (EXT), estimated (EST), calculated (CALC), and not applicable/available (N/A).)
DataTypeDescription	Text	A description of the data type (e.g., Experimental/Measured, Extrapolated, etc.)

The Synonyms table consists of fields to store information related to synonyms of the constituents. This table lists the CAS ID and a synonym for the chemical so that the database may be searched by any common or scientific name listed in the Constituents table or the Synonyms table. The table contains the fields shown and described in Table 43.

Table 43
Synonyms Table

FieldName	Data Type	Description
CasNo	Text	The Chemical Abstract Service Registry Number of the constituent
ConstituentName	Text	A synonym name of the constituent

Figures 9-15 show examples of the database "Constituents," "Parameters," "RangeValues," "Reference," "DataSource," "DataType," and "Synonyms" tables, respectively. Figure 16 shows the schema for the seven tables.

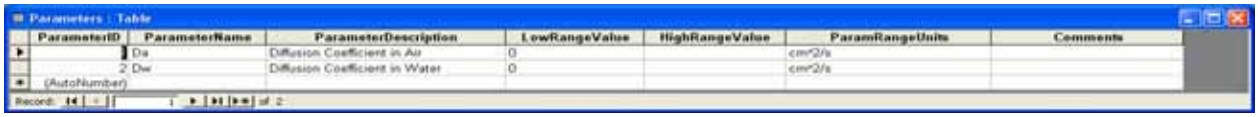


Constituents : Table

CasNo	ConstituentName	ConstituentClass
156-59-2	1,2-Dichloroethene (cis)	halogenated
156-60-5	1,2-Dichloroethene (trans)	halogenated
1074-11-9	(1,2-dichloroethyl) benzene	halogenated
95-63-6	1,2,4-Trimethylbenzene	hydrocarbons
107-06-2	1,2-Dichloroethane	halogenated
32768-54-0	1,2-Dichloro-3-methylbenzene	halogenated
540-59-0	1,2-Dichloroethene (cis/trans MIXTURE)	halogenated
108-67-8	1,3,5-Trimethylbenzene (MESITYLENE)	hydrocarbons
99-35-4	1,3,5-Trinitrobenzene	explosives
106-99-0	1,3-Butadiene	hydrocarbons
99-65-0	1,3-Dinitrobenzene	explosives
81-63-0	1,4-Diamino-2,3-dihydroanthraquinone (DDA) violet-dye mix	biocides/dyes
128-80-3	1,4-Di-p-toluidinoanthraquinone (PTA) Green 3	biocides/dyes
71-36-3	1-Butanol	alcohols/ketones
106-98-9	1-Butene	hydrocarbons
95-49-8	1-Chloro-2-methylbenzene	halogenated
108-41-8	1-Chloro-3-methylbenzene	halogenated
592-41-6	1-Hexene	hydrocarbons
109-67-1	1-Pentene	hydrocarbons
82-38-2	1-(Methylamino)anthraquinone (Disperse Red 9)	biocides/dyes
8003-22-3	2-(2-quinolinyl)-1,3-indandione (D & C yellow no. 11)	biocides/dyes
431-03-8	2,3-Butanedione	alcohols/ketones
1746-01-6	2,3,7,8-Tetrachlorodibenzo-p-Dioxin	furans+dioxins
118-96-7	2,4,6-Trinitrotoluene (TNT)	explosives
121-14-2	2,4-Dinitrotoluene (DNT; 2,4-DNT)	explosives
606-20-2	2,6-Dinitrotoluene (2,6-DNT)	explosives
625-86-5	2,5-Dimethylfuran	furans+dioxins
35572-78-2	2-Amino-4,6-Dinitrotoluene	explosives
117-79-3	2-amino-9,10-anthracenedione (a) (AAQ)	biocides/dyes
78-93-3	2-Butanone	alcohols/ketones
98-01-1	2-Furaldehyde	alcohols/ketones
110-43-0	2-Heptanone	alcohols/ketones
563-46-2	2-Methyl-1-butene	hydrocarbons
534-22-5	2-Methylfuran	furans+dioxins
554-14-3	2-Methylthiophene	hydrocarbons
88-72-2	2-Nitrotoluene (ONT)	explosives
107-87-9	2-Pentanone	alcohols/ketones

Record: 1 of 107

Figure 9. The “Constituents” database table

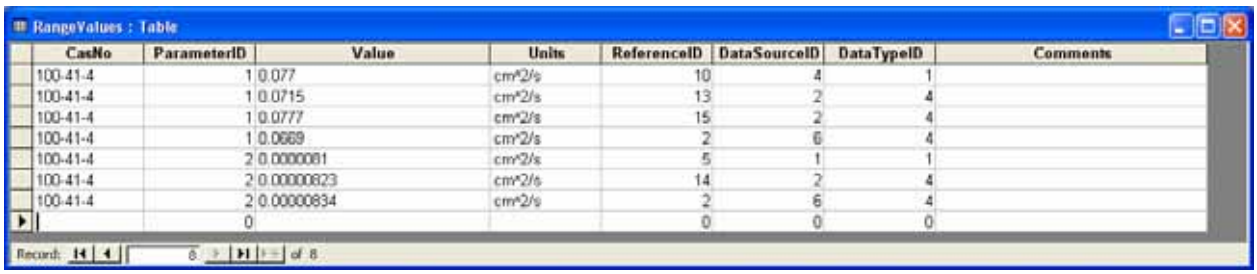


Parameters : Table

ParameterID	ParameterName	ParameterDescription	LowRangeValue	HighRangeValue	ParamRangeUnits	Comments
1	Da	Diffusion Coefficient in Air	0		cm^2/s	
2	Dw	Diffusion Coefficient in Water	0		cm^2/s	
(AutoNumber)						

Record: 1 of 2

Figure 10. The “Parameters” database table



RangeValues : Table

CasNo	ParameterID	Value	Units	ReferenceID	DataSourceID	DataTypeID	Comments
100-41-4	1	0.077	cm^2/s	10	4	1	
100-41-4	1	0.0715	cm^2/s	13	2	4	
100-41-4	1	0.0777	cm^2/s	15	2	4	
100-41-4	1	0.0669	cm^2/s	2	6	4	
100-41-4	2	0.0000081	cm^2/s	5	1	1	
100-41-4	2	0.00000823	cm^2/s	14	2	4	
100-41-4	2	0.00000834	cm^2/s	2	6	4	
	0			0	0	0	

Record: 4 of 8

Figure 11. The “RangeValues” database table

Figure 12. The “Reference” database table

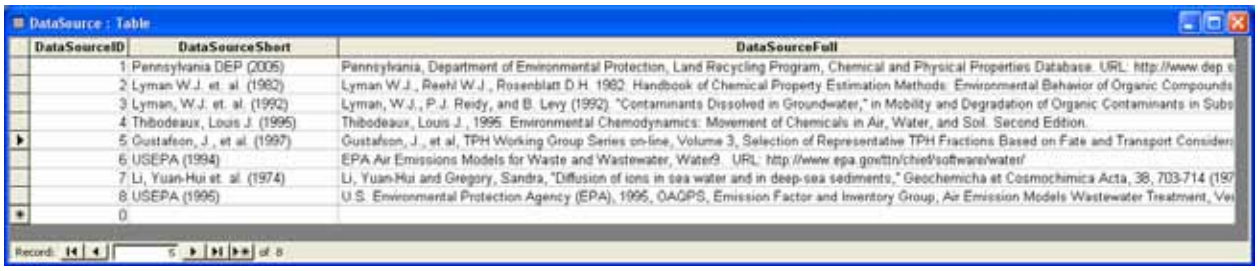


Figure 13. The “DataSource” database table

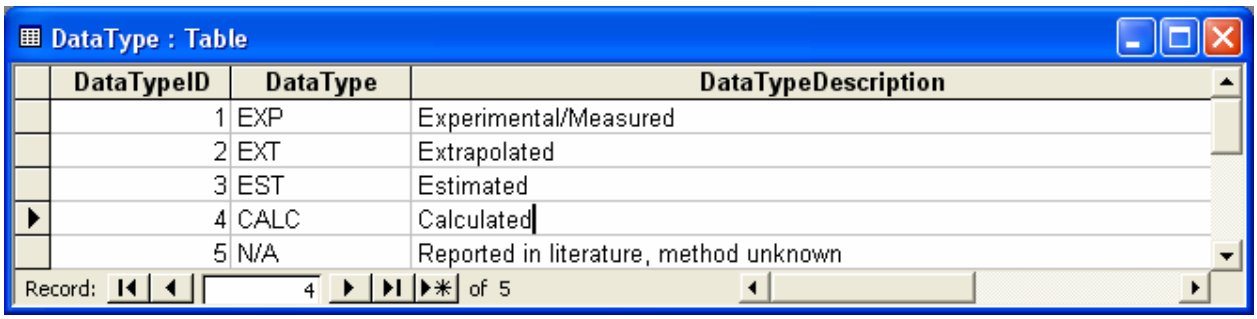


Figure 14. The “DataType” database table

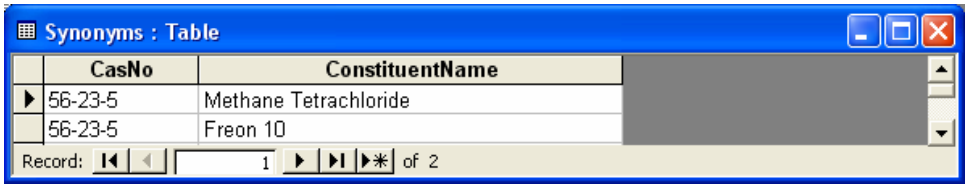


Figure 15. The “Synonyms” database table

This database format will allow the data to be more organized and easily accessible from the new interface or any program that requires access to the data, such as a database-client editor within ARAMS. It will also allow easier updates of the data as new information is acquired.

The data in the existing Range Database will first be migrated to the new database format. Then, the new data from the current study will be added to the new database. Finally, a new database browser interface will be written to facilitate viewing and retrieval of data.

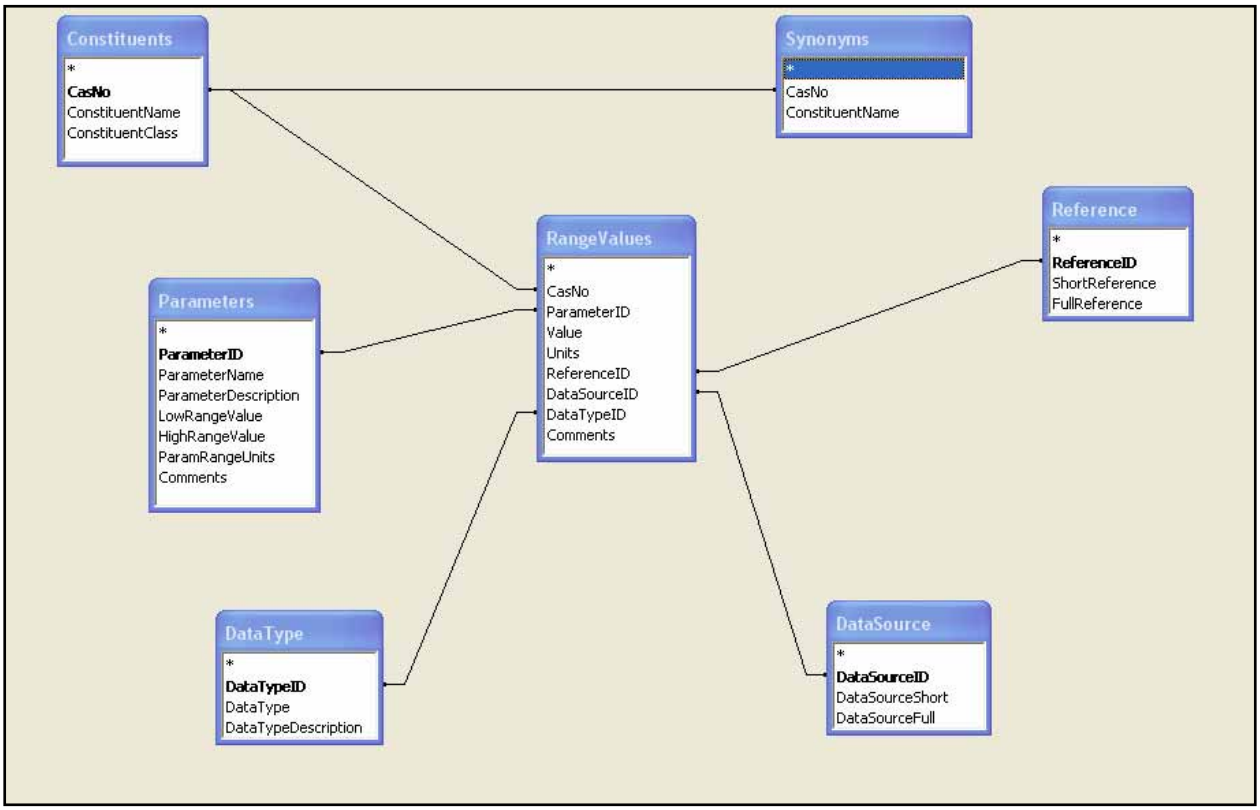


Figure 16. The Range Database schema

9 Summary of Conclusions and Recommendations

The objective of this study was to expand the Range constituent database to fill data gaps for properties and parameters required for fate/transport, human exposure, and human health effects assessment associated with 188 chemicals expected on Army and DoD training and firing ranges. In order to make significant progress on filling these gaps, it was necessary to use computational methods, extrapolation, and other means for estimating property/parameter values. Therefore, a major part of this study was devoted to evaluating and recommending various methods for predicting property/parameter values, then using such methods to generate estimates for the database. Objectives included documenting the accuracy of recommended estimation techniques, expansion of the database to include new values, documenting remaining data gaps, and recommending specific future research or testing to address remaining data gaps. The study focused on the following property/parameter categories:

- Physicochemical properties for fate and transport.
- Human exposure parameters.
- Food transfer factors.
- Environmental degradation rates.
- Human toxicological benchmarks.

A summary of conclusions and recommendations for each of the above categories follows below. Recommendations are explicitly restated in the second section of this chapter.

Conclusions

The physicochemical properties for fate/transport that were addressed in this study were: (1) molecular weight (MW), (2) octanol-water partition coefficient (K_{ow}), (3) water solubility, (4) vapor pressure, (5) Henry's law constant (HLC), and (6) molecular diffusivity in air and water. The MW was determined using the QB MW calculator, which uses the straightforward procedure of identifying the number and type of each atom found in the molecular structures in the database, multiplying the determined number of atoms by the appropriate atomic mass (for the naturally occurring isotopic distribution of each element), and

summing the products. The MW results compared very closely the values already in the Range Database.

The primary technique employed in providing estimates of values for properties (2) to (5), above, that were not otherwise available from the literature was the QSAR/QSPR. Comparison of the predicted values for these four properties against reference values indicated that reasonably accurate estimations for missing properties can be obtained. The average model error (AME) was less than 100 percent (i.e., within one order of magnitude of the reference values) for all four properties, whereas the range of values extended from about 12 to 20 orders of magnitude. Predictions were best for log HLC and log vapor pressure (AME of about 30 percent) and the poorest for log solubility (AME of about 94 percent). Further work on the inorganic species and select organic compounds with the development of fully optimized QSPR/QSAR tools is recommended.

Literature values for the diffusion coefficient in air were found for 35 of the 188 chemicals. For the diffusion coefficient in water, a total of 90 literature values were found. Missing values were calculated using various estimation equations presented in Chapter 3. Statistical analysis showed that the diffusion coefficient in air and water can generally be predicted quite well with an AME of less than 15 percent in most cases. Some classes of chemicals have higher AME values due to the nature of the chemicals in these classes. Results from all five methods (three for air and two for water) will be added to the Range Database along with the associated AME and average bias for each method and chemical class (because some estimation methods are more accurate than others for particular chemical classes). There were several chemicals for which diffusion coefficients could not be calculated. The methods do not work well for trace metals for which molar volume increments have not been determined. However, water diffusivity values in fresh water or seawater for all of the metals in particular valence states were found in the literature. Thus, all Range constituents have a diffusivity value for water. Additional research is not warranted for diffusivity values of the Range Database constituents.

Three human dermal exposure parameters were studied, aqueous skin permeability constant (K_p), GI absorption fraction (GI ABS), and dermal absorption fraction from soil (dermal ABS). Equation 15 is recommended for estimating K_p for organics if measured values are not available. The AME for Equation 15 was 73.6 percent for a select list of chemicals. Values of K_p were found in the literature for several inorganics (Table 11).

USEPA (2004b) reported values for GI ABS for a number of constituents (Table 12). Values for dermal ABS found in the literature are shown in Table 13. USEPA recommends default GI ABS values of 0.8 for volatile organics, 0.5 for semivolatile organics, and 0.2 for inorganic chemicals when measured values are not available. USEPA recommends using 0.001 for inorganic constituents and 0.01 for organics as default values for dermal ABS when specific data are not available. However, in some cases, the default values may overestimate dermal exposure.

Values are available in the ARAMS/FRAMES and RAIS Databases for K_p, GI ABS, and dermal ABS for a substantial number of Range Database constituents. Dermal ABS has the fewest number of values in the ARAMS/FRAMES Database. The RAIS Database has values for 111 Range Database constituents for all three parameters, but many of the values in the RAIS Database are default values rather than measured values.

Future studies should be considered to evaluate other empirical equations for estimating the aqueous skin permeability constant, such as Equation 16 and other types of models, such as the anatomically based, physical models. It appears that GI ABS should receive greater attention because values are not available for many compounds. For now, USEPA-recommended default values can be used in the absence of measured values. Of the three exposure parameters, the dermal ABS should probably receive the most attention in future research.

Few measured values are available for food transfer factors for the Range Database constituents. There are values in the RAIS Database for a substantial number of Range constituents, but many of these are estimated or default values. Many approaches are available to estimate food transfer factors for human exposure. The choice for the most appropriate method depends largely on the purpose of the risk assessment. For most purposes, it is often better to use a simple and generic empirical approach rather than a more demanding mechanistic one.

The variation in the different models for estimating food transfer factors can be quite large. There are very large data gaps for saltwater fish and aquatic plants. The empirical models for fish may be modified for a marine environment, but data are required for this. Thus, existing models must be used with caution for marine fish. The bulk of the consumed fish in the United States is retrieved from the marine water environment and not from the freshwater environment, although this situation may not apply for most Army exposure scenarios.

For bioaccumulation into meat and milk, large uncertainties should be expected. There is little room for improvement of the current approaches on the basis of the available data sets. For about 70 percent of the meat bioaccumulation factors, Travis and Arms used data based on concentrations in non-lactating cattle (Birak et al. 2001). An analysis has not yet been conducted to determine if there is a significant difference in the concentrations for the same chemical between lactating and non-lactating cattle. Further research is needed to determine whether the models of Dowdy et al. (1996) or McLachlan (1994) are a better alternative than the Travis and Arms approach. The Travis and Arms equations predict an increase in the concentrations in milk and meat with increasing log K_{ow}. This may greatly overestimate the concentration in milk and meat, because for high log K_{ow} compounds (log $K_{ow} > 6$), the bioaccumulation factors have been found to decrease. The fat content of meat used for the Travis and Arms correlation is rather high. All milk products are represented by milk, which is not valid for the much fattier milk products like cheese and butter. Perhaps it is better to relate concentrations in meat and milk to fat content. Also, cattle were not exposed to other fodder types, other than grass. Due to this assumption, the model calculations represent a conservative situation since the

concentration in other fodder may be significantly lower than in grass. Until another more reliable method is provided, the Travis and Arms equations will be used to estimate meat and milk BTFs for organic chemicals in the Range database. For inorganics, Ba_{beef} and Ba_{milk} values may be obtained from Baes et al. (1984) (See Figures 2 and 3).

Overall, there is much work to be done in determining food transfer factors given the variability in predictive methods and the lack of predictive relationships for some food types. The methods recommended for filling in (populating) the Range Database food transfer factors for now are presented in Table 22.

There have been many publications of degradation rates of chemical compounds in the environment. However, even for well-studied compounds, there is often disagreement in publications as to the values of the degradation rates, even under similar environmental conditions. Thus, there are many data gaps for degradation rates, so QSAR software packages were examined that could be predictive of environmental degradations rates. Two QSAR programs were examined, the Estimation Programs Interface (EPI) Suite, and the Persistence Bioaccumulation Toxicity (PBT) Profiler. EPI provided results for all 188 compounds, whereas PBT does not output certain data for metallic elements and for some compounds that lack effective organic functional groups. For those chemicals for which PBT caveats yield no results, the EPI results are suspect too for the same reasons given in the PBT documentation. In general the degradation rates for a particular media or process are either filled in for all constituents in the database or are empty for all the compounds in the database due to the assumptions and limitations of the software. However, the predicted values are quite uncertain. Estimated half-lives for air, water, and soil were compared to reported values, and the accuracy of estimates was evaluated. The errors were very large, where AME was on the order of thousands of percent, and large negative average bias was found, which means that the half-lives are under-predicted, leading to more rapid predicted degradation and, therefore, lower predictions of environmental exposure concentrations (i.e., lack of persistence).

There remain important gaps for process-specific degradation rates, especially hydrolysis and photolysis in water. The results of the analysis suggest improvements that could be made in the predictions. It was expected that rates of reaction in the environment would be too difficult to predict accurately for all compounds under all conditions. Of most immediate use would be modifications of the fits used to develop the current models to more accurately fit the data for air, soil, and water for the compounds in the Range Database. Separately, software packages could be developed that calculate rates of hydrolysis and photolysis of water.

Degradation rates are likely to remain highly uncertain. As noted previously, measuring degradation rates is costly and problematic because such rates are highly site- and chemical-specific. Field measurements and/or controlled laboratory experiments (with field-like conditions) should be coupled to more accurately determine rates. Future research in this area should include improving the predictive QSAR models. In the interim, conservative assumptions should be

used in exposure assessment, i.e., long half-lives and high persistence in the environment.

A hierarchy was followed to address gaps in human toxicological benchmarks. Initially, all substances were checked for the existence of chronic toxicity benchmarks (noncancer and cancer). If no benchmarks existed, then the literature was evaluated to determine if, at a minimum, any subchronic or chronic animal studies of sufficient quality were available. If so, these data were used to derive Reference Dose (RfD) and Reference Concentration (RfC) equivalent values. If sufficient subchronic or chronic data were not available, then chemical structure was available to derive an RfD surrogate using the QSAR approach and the TOPKAT software. When these relationships were weak, the recommended tests needed to develop the appropriate chronic benchmark were suggested.

Oral RfD, inhalation RfD, or both, were found for 94 constituents in the overall Range constituent list. Of the 94 constituents without published RfDs, provisional estimates of the oral RfD were made on most (72 constituents). Published subchronic data or benchmark allowed for a derivation of an Rfd for 28 of 72 compounds. In the remaining 44 cases, the RfD estimate was derived solely from QSAR estimates, primarily of the estimated rat chronic LOAEL derived for each compound in question or a surrogate compound. The confidence in the estimate is "high" or "medium" in the case of 34 of these 44 constituents.

Of the remaining 22 constituents out of 94 without published RfD values, 4 were strongly carcinogenic (therefore derivations of noncarcinogenic values were meaningless); 6 were simple asphyxiants; 5 included compounds that were either mixed isomers or no usable basis for derivation was possible; and 7 were inorganic compounds or metals (thus the QSAR approach was invalid). Provisional RfD estimates were not attempted on the latter because the TOPKAT system does not encompass metals, inorganics, or organometallics.

The ten compounds having estimates of provisional RfD that were based on QSAR estimates where the confidence in the estimate is of low reliability are:

Compound	CAS Number
1,4-Di-p-toluidino anthraquinone	(128-80-3)
Isothiocyanato methane	(556-61-6)
o-Methoxy-phenylazo-b-naphthol	(1229-55-6)
Carbonyl sulfide	(463-58-1)
Indeno(1,2,3,cd) pyrene	(193-39-5)
Phenylacetylene	(536-74-3)
trans-3-Penten-2-one	(3102-33-8)
Methylnitrite	(624-91-9)
1,4-Diamino-2,3-dihydroanthraquinone	(81-63-0)
3-Methyl-1-butene	(563-45-1)

It is recommended that these compounds be considered for possible subchronic toxicity testing, after consideration of other factors such as human

exposure potential. Subchronic in-vivo (rodent) toxicity testing is also recommended for at least 10 compounds for which RfDs or RfD-equivalent values could not be developed. Subchronic toxicity testing is necessary to develop benchmarks for several constituents; however, the prioritization for such tests rests on the magnitude of exposure (exposure potential) and confidence in available toxicity data. In certain circumstances it may be advisable to conduct a focused test on a substance found in significant quantities with a highly uncertain QSAR estimate rather than to fill a toxicological data gap for a substance that has very limited exposure potential. The priority of such studies, however, should be considered based on the magnitude of exposure and best professional judgment.

Thirty-nine substances had reported cancer slope factors (CSFs). Cancer classifications or cancer groups were found for 67 of the substances not having CSFs. Testing for cancer should involve a tiered approach, whereby in-vitro screening precedes animal testing. This testing should be based on priority of cancer groupings and prevalence of the substance in the environment.

In summary, many property/parameter gaps for the Range Database constituents have been filled using estimation techniques. However, the error of such estimates can be quite large, as in the case of environmental degradation rates, or half-lives. Although degradation rates are highly uncertain, the use of conservative values (i.e., persistence in the environment) and refinement of QSAR models are recommended for the near term. Other estimates can be quite good, as is the case of physicochemical properties for fate/transport. Although estimation techniques work quite well for physicochemical properties, some refinement of the models is recommended for inorganics and several organic compounds. As for human exposure factors, dermal ABS should be given the greatest consideration for future study. Although a variety of estimation techniques exist for food transfer factors, accuracy is a concern. There are essentially no estimation methods and little observed data for aquatic plant and marine animal food transfer factors, and further study is warranted. Human toxicological benchmarks exist for many of the Range constituents, even if only provisional values at this time.

Recommendations

This section explicitly lists recommendations for future study and/or research to address remaining data gaps in constituent properties/parameters. Recommendations for each parameter category are addressed separately for clarity.

Physicochemical properties for fate and transport

Although estimation techniques work quite well for physicochemical properties, some refinement of the models is recommended for inorganics and several organic compounds through development of more fully optimized QSPR/QSAR tools. Additional research is not warranted for diffusivity values of the Range Database constituents.

Human exposure parameters

Equation 15 and Tables 12, 14, and 15 are recommended for now for estimating aqueous skin permeability when measured values are not available. The default value for inorganic chemicals lacking values is 10^{-3} cm/hr. Future studies should be considered to evaluate other empirical equations for estimating the aqueous skin permeability constant, such as Equation 16 and other types of models, such as the anatomically based, physical models

Tables 12, 14, and 15 are recommended for values of GI ABS. USEPA recommends default GI ABS values of 0.8 for volatile organics, 0.5 for semi-volatile organics, and 0.2 for inorganic chemicals when measured values are not available. Additional study is recommended for GI ABS since values are not available for many compounds. For now, USEPA-recommended default values can be used in the absence of measured values.

Tables 13, 14, and 15 are recommended for values of dermal ABS. USEPA recommends using 0.001 for inorganic constituents and 0.01 for organics as default values for dermal ABS when values are not available. However, in some cases, the default values may overestimate dermal exposure.

Of the above three exposure parameters, the dermal ABS should probably receive the most attention in future Army research since this parameter has the most data gaps and is also less likely to be addressed by other agencies such as USEPA, especially for military relevant constituents.

Food transfer factors

Study of bioaccumulation differences between lactating and non-lactating cattle is recommended. Further research is needed to determine whether the models of Dowdy et al. (1996) or McLachlan (1994) are a better alternative than the Travis and Arms approach. There should be an investigation of using fat content to predict meat and milk concentrations. Study of cattle exposed to other fodder types, other than grass, is recommended. Until other, more reliable methods are provided, the Travis and Arms equations should be used to estimate meat and milk food transfer factors for organic chemicals. For inorganic chemicals, Ba_{beef} and Ba_{milk} values may be obtained from Baes et al. (1984) (see Figures 2 and 3).

Table 22 lists the recommended equations, tables, and figures within this report for estimating various types of food transfer factors. There are essentially no estimation methods and little observed data for aquatic plant, freshwater shellfish, and marine animal food transfer factors; thus, much further study is recommended for these.

Environmental degradation rates

It is recommended that the fits used to develop the current models for degradation rates in air, soil, and water be improved to more accurately predict rates for the compounds in the Range Database. Additionally, it is recommended that other software packages be explored for calculating rates of hydrolysis and photolysis in water.

Field measurements and/or controlled laboratory experiments (with field-like conditions) should be used to more accurately determine rates. Additionally, future research in this area should include improving the predictive QSAR models. In the interim, conservative assumptions should be used in exposure assessment, i.e., long half-lives and high persistence in the environment.

Human toxicological benchmarks

It is recommended that the following 10 compounds be considered for possible subchronic toxicity testing, after consideration of other factors such as human exposure potential:

Compound	CAS Number
1,4-Di-p-toluidino anthraquinone	(128-80-3)
Isothiocyanato methane	(556-61-6)
o-Methoxy-phenylazo-b-naphthol	(1229-55-6)
Carbonyl sulfide	(463-58-1)
Indeno(1,2,3,cd) pyrene	(193-39-5)
Phenylacetylene	(536-74-3)
trans-3-Penten-2-one	(3102-33-8)
Methylnitrite	(624-91-9)
1,4-Diamino-2,3-dihydroanthraquinone	(81-63-0)
3-Methyl-1-butene	(563-45-1)

Subchronic in vivo (rodent) toxicity testing is also recommended for at least 10 compounds for which RfDs or RfD-equivalent values could not be developed. Subchronic toxicity testing is necessary to develop benchmarks for several constituents as discussed in Chapter 7; however, the prioritization for such tests rests on the magnitude of exposure (exposure potential) and confidence in available toxicity data. In certain circumstances it may be advisable to conduct a focused test on a substance found in significant quantities with a highly uncertain QSAR estimate rather than to fill a toxicological data gap for a substance that has very limited exposure potential. The priority of such studies, however, should be considered based on the magnitude of exposure and best professional judgment.

Testing for cancer should involve a tiered approach, whereby in vitro screening precedes animal testing. This testing should be based on priority of cancer groupings and prevalence of the substance in the environment.

References

Aberg, B., Ekman, L., Falk, R., Greitx, U., Persson, G., and Snihs, J. (1969). "Metabolism of methyl mercury (203 Hg) compounds in man," *Arch Environ. Health* 19, 453-484.

Agency for Toxic Substances and Disease Registry. (1994a). "Toxicological profile for chlorodibenzofurans," U.S. Department of Health and Human Services, Public Health Service.

_____ . (1994b). "Toxicological profile for mercury," U.S. Department of Health and Human Services, Public Health Service.

_____ . (1994c). "Toxicological profile for zinc," U.S. Department of Health and Human Services, Public Health Service.

_____ . (2001). "Online minimal risk levels for hazardous substances," U.S. Department of Health and Human Services, Public Health Service.

Albro, P. W., and Fishbein, L. (1972). "Intestinal absorption of polychlorinated biphenyls in rats," *Bull. Environ. Contam. Toxicology* 8, 26-31.

American Conference of Governmental Industrial Hygienists. (1999). "Documentation of the threshold limit values and biological exposure indices," American Conference of Governmental Hygienists, Inc., Cincinnati, OH.

American Industrial Hygiene Association. (2001). "Emergency response planning guidelines and workplace environmental exposure level guides handbook," Fairfax, VA.

Atkinson, R. (1985). "Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds under atmospheric conditions," *Chem. Rev.* 85, 69-201.

_____ . (1986). "Estimations of OH radical rate constants from H-atom abstraction from C-H and O-H bonds over the temperature range 250-1000 K," *Intern. J. Chem. Kinet.* 18, 555-568.

Atkinson, R. (1987). "A structure-activity relationship for the estimation of rate constants for the gas-phase reactions of OH radicals with organic compounds," *Intern. J. Chem. Kinet.* 19, 799-828

_____ . (1988). "Estimation of gas-phase hydroxyl radical rate constants for organic chemicals," *Environ. Toxicol. Chem.* 7, 435-442.

_____ . (1989). "Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds," *J. Phys. Chem. Ref. Data* Monograph No. 1, Amer. Inst. Physics and Amer. Chem Soc., New York.

_____ . (1991). "Kinetics of the gas-phase reactions of a series of organosilicon compounds with OH and NO3 radicals and O3 at 297 ± 2K," *Environmental Science and Technology* 25, 863-6.

Atkinson, R., and Aschmann, S. M. (1992). "OH radical reaction rate constants for polycyclic alkanes: Effects of ring strain and consequences for estimation methods," *Intern. J. Chem. Kinetics* 24, 983-9.

Atkinson, R., and Carter, W. P. L. (1984). "Kinetics and mechanisms of the gas-phase reactions of ozone with organic compounds under atmospheric conditions," *Chemical Reviews* 84, 437-70.

Bacci, E., Cerejeira, M. J., Gaggi, C., Chemello, G., Calamari, D., and Vighi, M. (1990). "Bioconcentration of organic chemical vapors in plant leaves: The azalea model," *Chemosphere* 21, 4-5.

_____ . (1992). "Chlorinated dioxins: Volatilization from soils and bioconcentration in plant leaves," *Bulletin of Environmental Contamination and Toxicology* 48(3), 401-408.

Baes, C. F., III, Sharp, R. D., Sjoreen A. L., and Shor, R. W. (1984). "A review and analysis of parameters for assessing transport of environmentally released radionuclides through agriculture," ORNL-5786, Oak Ridge National Laboratory.

Barron, M. G. (1990). "Bioconcentration: Will water-borne organic chemicals accumulate in aquatic animals?" *Environmental Science and Technology* 24(11)

Bettley, F. R., and O'Shea, J. A., (1975). "The absorption of arsenic and its relation to carcinoma," *Brit. J. Dermatol.* 92, 563-568.

Biermann, H. W., MacLeod, H., Atkinson, R., Winer,A. M., and Pitts, J. N., Jr. (1985). "Kinetics of the gas-phase reactions of the hydroxyl radical with naphthalene, phenanthrene, and anthracene," *Environmental Science and Technology* 19, 244-248.

Bintein, S., Devillers, J., and Karcher, W. (1993). "Nonlinear dependence of fish bioconcentration on n-octanol/water partition coefficient," *SAR QSAR Environmental Research* 1, 29-39.

Birak, P., Yurk, J., Adeshina, F., Lorber, M., Pollard, K., Choudhury, H., and Kroner, S. (2001). "Travis and Arms revisited: A second look at a widely used bioconcentration algorithm," *Toxicol. Ind. Health*. 17(5-10), 163-75.

Boethling, R. S., and Sabljic, A. (1989). "Screening-level model for aerobic biodegradability based on a survey of expert knowledge," *Environmental Science and Technology* 23, 672-9.

Boethling, R. S., Howard, P. H., Meylan, W. M., Stiteler, W., Beauman, J., and Tirado, N. (1994). "Group contribution method for predicting probability and rate of aerobic biodegradation," *Environmental Science and Technology* 28, 459-65.

Briggs, G. G., Bromilow, R. H., and Evans, A. A. (1982). "Relationships between lipophilicity and root uptake and translocation of non-ionized chemicals by barley," *Pesticide Science* 13, 495-504.

Calamari, D., Vighi, M., and Bacci, E. (1987). "The use of terrestrial plant biomass as a parameter in the fugacity model," *Chemosphere* 16(l0-12), 2359-2364.

California Environmental Protection Agency. (2000). "Technical support document for exposure assessment and stochastic analysis," Office of Environmental Health Hazard Assessment, Oakland, CA.

_____ . (2004). "Toxicity criteria database," Office of Environmental Health Hazard Assessment, Sacramento, CA. Online database: http://www.oehha.ca.gov/risk/ChemicalDB/start.asp

Chang, L. H. (1943) "The fecal excretion of polycyclic hydrocarbons following their administration to the rat," *J. Biochemistry* 151, 93-99.

Chrostowski, P. C., and Foster, S. A. (1996). "A methodology for assessing congener-specific partitioning and plant uptake of dioxins and dioxin-like compounds," *Chemosphere* 32(11), 2285-2304.

Conklin, A. W., Skinner, S. C., Felten, T. L., and Sanders, C. L. (1982). "Clearance and distribution of intratracheally instilled vanadium compounds in the rat," *Toxicol. Lett.* 11, 199-203.

Connell, D. W., and Hawker, D. W. (1988). "Use of polynomial expressions to describe the bioconcentration of hydrophobic chemicals by fish," *Ecotoxicol. Environ. Saf.* 16(3), 242-57.

Cuddihy, R. G., and Griffith, W. C. (1972). "A biological model describing tissue distribution and whole-body retention of barium and lanthanum in beagle dogs after inhalation and gavage," *Health Phys.* 23, 621-633.

Davidsson, L., Cederblad, A., Lonnerdal, B., and Sandstrom, B. (1989). "Manganese retention in man: A method for estimating manganese absorption in man," *Am. J. Clin. Nutr.* 49, 170-179.

Dean, J. A. (ed.). (1985). *Lange's handbook of chemistry.* 13th ed., McGraw-Hill Book Company, New York, 3-133 to 3-138.

Dean, J. A. (1987). *Handbook of organic chemistry.* McGraw-Hill Book Company, New York, 7-1 to 7-7.

Devillers, J., Bintein, S., and Domine, D. (1996). "Comparison of BCF models based on log P," *Chemosphere* 33(6), 1047-1065.

Devillers, J., Domine, D., Bintein, S., and Karcher, W. (1998). "Fish bioconcentration modeling with log P," *Toxicol. Methods* 8(1), 1-10.

Donaldson, R. M., and Barreras, R. F. (1996). "Intestinal absorption of trace quantities of chromium," *J. Lab. Clin. Med*. 68, 484-493.

Dowdy, D. L., McKone, T. E., and Hsieh, D. P. H. (1996). "Prediction of chemical biotransfer of organic chemicals from cattle diet into beef and milk using the molecular connectivity index," *Environmental Science and Technology* 30(3), 984-989.

Duff, R. M., and Kissel, J. C. (1996). "Effect of soil loading on dermal absorption efficiency from contaminated soils," *J. Tox. and Environ. Health* 48, 93-106.

Elakhovskaya, N. P. (1972). "The metabolism of nickel entering the organism with water," (Russian translation) *Gig Sanit* 6, 20-22.

Ewing, A. D., Kadry, A. M., and Dorough, H. W. (1985). "Comparative disposition and elimination of chlordane in rats and mice," *Toxicol. Lett.* 26, 233-239.

Farooqui, M. Y. H., and Ahmed, A. E. (1982). "Molecular interaction of acrylonitrile and potassium cyanide with rat blood," *Chem. Biol. Interact*. 38, 145-159.

Flynn, G. L. (1990). "Physiochemical determinants of skin absorption." *Principles of route-to-route extrapolation for risk assessment*. T.R. Gerity, C. J. Henry, ed., Elsevier Science Publishing Co. Inc., Amsterdam, 93-127.

Fries, G. F., and Marrow, G. S. (1975). "Retention and excretion of 2,3,7,8-tetrachlorodibenzo-p-dioxin by rats," *J. Agric. Food Chem*. 23, 265.

Fryer, M. E., and Collins, C.D. (2003). "Model intercomparison for the uptake of organic chemicals by plants," *Environmental Science and Technology* 37(8), 1617-24.

Fuller, E. N., Schettler, P. D., and Giddings, J.C. (1966). "A new method for prediction of binary gas-phase diffusion coefficients," *Ind. Eng. Chem.* 58, 19-27.

Furchner, J. E., Richmond, C. R., and Drake, G. A. (1968). "Comparative metabolism of radionuclides in mammals-IV. Retention of silver-110m in the mouse, rat, monkey, and dog," *Health Phys*. 6, 505-14.

Gobas, F. A. P. C. (1993). "Gastrointestinal magnification: The mechanism of biomagnification and food chain accumulation of organic chemicals," *Environmental Science and Technology* 27(13), 2855-63.

Gobas, F. A. P. C., and Morrison, H.A. (2000). "Bioconcentration and biomagnification in the aquatic environment." *Handbook of property estimation methods for chemicals*. R. S. Boethling and D Mackay, ed., Lewis Publishers, CRC Press LLC.

Goodman, M. A., Aschmann, S. M., Atkinson, R. and Winer, A. M. (1988). "Atmospheric reactions of a series of dimethyl phosphoroamidates and dimethyl phosphorothioamidates," *Environmental Science and Technology* 22, 578-83.

Gustafson, J., Tell, J. T., and Orem, D. (1997). "Selection of representative TPH fractions based on fate and transport considerations," TPH Working Group Series on-line, Vol 3, http://www.aehs.com/publications/catalog/contents/tph.htm

Guy, R. H., and Hadgraft, J. (1989). "Structure-activity correlations in percutaneous absorption." *Percutaneous absorption*. R. L. Bronaugh and H. I. Maibach, ed., Marcel Dekker, New York, 95-109.

Hansch, C., and Leo, A. J. (1979). *Substituent constants for correlation analysis in chemistry and biology.* John Wiley & Sons, New York.

Harris, J. C., and Hayes, M. J. (1990). "Acid dissociation constant." *Handbook of chemical property estimation methods*. W. J. Lyman, W. F. Reehl, and D. H. Roseblatt, ed., American Chemical Society, Washington, DC, 6-10 - 6-14.

Hayduk, W., and Laudie, H. (1974). "Prediction of diffusion coefficients for non-electrolysis in dilute aqueous solutions," *AIChe J.* 20, 611-15.

Hecht, S. S., Grabowski, W., and Groth, K. (1979). "Analysis of faeces for benzo[a]pyrene after consumption of charcoal-broiled beef by rats and humans," *Cosmet. Toxicology* 17, 223-227.

Hostynek, J. J., Hinz, R. S, Lorence, C. R, and Guy, R. H. (1998). "Human skin penetration by metal compounds." *Dermal absorption and toxicity assessment*. M. S. Roberts and K. A. Walters, ed., Marcel Dekker, Inc., NewYork.

Howard, P. H., Boethling, R. S., Stiteler, W. M., Meylan, W. M., Hueber, A. E., Beauman, J. A., and Larosche, M.E. (1992). "Predictive model for aerobic biodegradability developed from a file of evaluated biodegradation data," *Environ. Toxicol. Chem*. 11, 593-603.

Howard, P. H., Hueber, A. E., and Boethling, R. S. (1987). "Biodegradation data evaluation for structure/biodegradability relations," *Environ. Toxicol. Chem.* 6, 1-10.

Hung, H., and Mackay, D. (1997). "A novel and simple model of the uptake of organic chemicals by vegetation from air and soil," *Chemosphere* 35(5), 959-77.

Jager, D. T., and Hamers, T. (1997). "Estimation methods for bioaccumulation in risk assessment of organic chemicals," RIVM Report 679102013, National Institute for Public Health and the Environment, Bilthoven, Netherlands.

Jager, D. T., and Slob, W. (1995). "Uncertainty analysis of the uniform system for the evaluation of substances (USES)," RIVM Report 679102027, National Institute for Public Health and the Environment, Bilthoven, Netherlands.

Jager, D. T., Rikken, MG. J., and van der Poel, P. (1997). "Uncertainty analysis of EUSES: Improving risk management by probabilistic risk assessment," RIVM Report 679102039, National Institute for Public Health and the Environment, Bilthoven, Netherlands.

Japertas, P., Didziapetris, R., and Petrauskas, A. (2002). "Fragmental methods in the design of new compounds. Applications of the advanced algorithm builder," *Quant. Struct.-Act. Relat*. 21, 23-37.

Jarvis, M. W., and Lugg, G. A. (1968). "The calculation of diffusion coefficients of vapors of liquids into air," Report 318, Australian Defense Scientific Service, Alexandria, VA, 33.

Kasting, G. B., Smith, R. L., and Cooper, E. R. (1987). "Effect of lipid solubility and molecular size on percutaneous absorption," *Pharmacol. Skin* 1, 138-153.

Keim, K. S., Holloway, C .L., and Hebsted, M. (1987). "Absorption of chromium as affected by wheat bran," *Cereal Chem.* 64, 352-355.

Keller, W., and Yeary, R. (1980). "A comparison of the effects of mineral oil, vegetable oil, and sodium sulfate on the intestinal absorption of DDT in rodents," *Clin. Toxicol*. 16, 223-231.

Klöpffer, W., and Kohl, E. G. (1993). "Bimolecular OH rate constants of organic compounds in solution," *Ecotox. Environ. Safety* 26, 346-356.

Knopp, D., and Schiller, F. (1992). "Oral and dermal application of 2,4-dichlorophenoxyacetic acid sodium and dimethylamine salts to male rats: Investigations on absorption and excretion as well as induction of hepatic mixed-function oxidase activities," *Arch Toxicol.* 66, 170-174.

Korte, F. (1978). "Ecotoxicologic profile analysis," *Chemisphere* 1, 79-102.

Kwok, E. S. C., and Atkinson, R. (1995). "Estimation of hydroxyl radical reaction rate constants for gas-phase organic compounds using a structure-reactivity relationship: An update," *Atmospheric Environment* 29, 1685-1695.

Kwok, E. S. C., Aschmann, S. M., and Atkinson, R. (1996). "Rate constants for the gas-phase reaction of selected carbamates and lactates," *Environmental Science and Technology* 30, 329-334.

Kwok, E. S. C., Atkinson, R., and Arey, J. (1992). " Gas-phase atmospheric chemistry of selected thiocarbamates," *Environmental Science and Technology* 26, 1798-1807.

Leahy, D. E. (1990). "Use of QSAR's to predict percutaneous absorption." *Prediction of percutaneous penetration*. R. C. Scott, R. H. Guy, and J. Hadgraft, ed., IBC Technical Services Ltd, London, 242-251.

Leifer, A. (1993). "Determination of rates of reaction in the gas-phase in the troposphere. Theory and practice. 5. Rate of indirect photoreaction," EPA/744/R-93/001 (NTIS PB93-149334), U.S. Environmental Protection Agency, OPPT, Washington, DC.

Li, Y-H., and Gregory, S. (1974). "Diffusion of ions in sea water and in deep-sea sediments," *Geochemicha et Cosmochimica Act* 38, 703-714.

Lide, D. R., ed. (1997). *CRC handbook of chemistry and physics*. 78th ed., CRC Press.

Lie, R., Thomas, R. G., and Scot, J. K. (1960). "The distribution and excretion of thallium 204 in the rat suggested MPCs and a bioassay procedure," *Health Phys*. 2, 334-340.

Lien, E. J., and Tong, G. L. (1973). "Physicochemical properties and percutaneous absorption of drugs," *J. Soc. Cosmet. Chem.* 24, 371-384.

Lu, X., Tao, S., Cao, J., and Dawson, R. W. (1999). "Prediction of fish bioconcentration factors of nonpolar organic pollutants based on molecular connectivity indices," *Chemosphere* 39(6), 987-999.

Lu, X., Tao, S., Hu, H., and Dawson, R.W. (2000). Estimation of bioconcentration factors of nonionic organic compounds in fish by molecular connectivity indices and polarity correction factors. *Chemosphere* 41(10), 1675-88.

Lugg, G. A. (1968). "Diffusion coefficients of some organic and other vapors in air," *Anal. Chem.* 40, 1072-1077.

Lyman, W. J., Reehl, W. F., and Rosenblatt, D. H. (1982a). *Handbook of chemical property estimation methods*. McGraw-Hill Book Company, New York.

Lyman, W. J., Reehl, W. J., and Rosenblatt, D. H. (1982b). *Handbook of chemical property estimation methods: Environmental behavior of organic compounds*. McGraw-Hill, New York.

Lyman, W. J., Reidy, P. J., and Levy, B. (1992). "Contaminants dissolved in groundwater." *Mobility and degradation of organic contaminants in subsurface environments.* C.K. Smoley, Inc., Chelsea, MI, 207-235.

Mabey, W., and Mill, T. (1978). "Critical review of hydrolysis of organic compounds in water under environmental conditions," *J. Phys. Chem. Ref. Data* 7(2), 383-415.

Mackay, D. (1982). "Correlation of bioconcentration factors," *Environmental Science and Technology* 16, 274-278.

Mackay, D., and Fraser, A. (1982). "Correlation of bioconcentration factors," *Environmental Science and Technology* 16, 274-278.

_____ . (2000). "Bioaccumulation of persistent organic chemicals: Mechanisms and models," *Environ. Pollut*. (Oxford, U. K.) 110(3), 375-391.

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

Mackenzie, R. D., Anwar, R. A., Byerrum, R. U., and Hoppert, C. A. (1959). "Absorption and distribution of Cr 51 in the albino rat," *Arch. Biochem. Biophys.* 79, 200-205.

MacPhee, J. A., Panaye, A., and Dubois, J. (1978). "A critical examination of the Taft Steric Parameter-Es. Definition of a revised, broader and homogeneous scale. Extension to highly congested alkyl groups," *Tetrahedron* 34, 3553-3562.

Macrady, J. K., and Maggard, S.P. (1993). "Uptake and photodegradation of 2,3,7,8-tetrachlorodibenzo-p-dioxin sorbed to grass foliage," *Environmental Science and Technology* 27, 343-350.

Mannhold, R., and Dross, K. (1996). "Calculation procedures for molecular lipophilicity: A comaparative study," *Quant. Struct.-Act. Relat.* 15, 403-409.

McKone, T. E. (1993). "CalTOX, A multimedia total exposure model for hazardous-waste sites," UCRL-Cr-111456, Lawrence Liverpool National Laboratory, Liverpool, CA.

McKone, T. E., and Howd, R. A. (1992). "Estimating dermal uptake of nonionic organic chemicals from water and Soil; Part 1, Unified fugacity-based models for risk assessments," *Risk Analysis* 12, 543-557.

McLachlan, M. S. (1994). "Model of the fate of hydrophobic contaminants in cows," *Environmental Science and Technology* 28(13), 2407-2414.

_____ . (2000). "Vegetation–air partition coefficient." *Handbook of property estimation methods for chemicals*. R. S. Boethling and D. Mackay ed., CRC, Boca Raton, FL, 115-123.

McLachlan, M. S., Thoma, H., Reissinger, M., and Hutzinger, O. (1990). "PCDD/F in an agricultural food chain, Part I, PCDD/F mass balance of a lactating cow," *Chemosphere* 20(7-9), 1013-1020.

Meerman, J. H., Sterenborg, H. M., and Mulder G. J. (1983). "Use of pentachlorophenol as long-term inhibitor of sulfation of phenols and hydroaximic acids in the rat in-vivo," *Biochem. Pharmacol.* 32, 1587-1593.

Meylan, W. M., and Howard, P. H. (1993). "Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone," *Chemosphere* 26, 2293-2299.

Meylan, W. M., Howard, P. H., Boethling, R. S., Aronson, D., Printup, H., and Gouchie, S. (1999). "Improved method for estimating bioconcentration/ bioaccumulation factor from octanol/water partition coefficient," *Environmental Toxicology and Chemistry* 18(4), 664-672.

Mill, T., Haag, W., Penwell, P., Pettit, T., and Johnson, H. (1987). "Environmental fate and exposure studies development of a PC-SAR for hydrolysis: Esters, alkyl halides and epoxides," EPA Contract No. 68-02-4254, SRI International, Menlo Park, CA.

Montgomery, J. H. (1996). *Groundwater chemicals desk reference*. 2nd ed., Lewis Publishers.

Mount, G. H., and Eisele, F. L. (1992). "An intercomparison of tropospheric OH measurements at Fritz Peak Observatory, Colorado," *Science* 256, 1187-1188.

Muhlebach, S. (1981). "Pharmacokinetics in rats of 2,4,5,2,4,5 hexachlorobi-phenyl and unmetabolizable lipophilic model compounds," *Xenobiotica* 11, 249-257.

Müller, J. F., Hawker, D. W., and Connell, D. W. (1994). "Calculation of bioconcentration factors of persistent hydrophobic compounds in the air/vegetation system," *Chemosphere* 29, 623-640.

National Toxicology Program. (1990). "Toxicology and carcinogenesis studies of furfural in F344/N rats and B6C3F1 mice (gavage studies)," *National Toxicology Program Technical Report Series* 382.

Neely, B. W., Branson, D. R., and Blau, G. E. (1974). "Partition coefficient to measure bioconcentration potential of organic chemicals in fish," *Environmental Science and Technology* 8, 1113-1115.

Ohno, Y., Kawanishi, T., and Takahashi, A. (1986). "Comparisons of the toxicokinetic parameters in rats determined for low and high dose gamma-chlordane," *J. Toxicol. Sci.* 11, 111-124.

Paterson, S., and Mackay, D. (1994). "A model of organic chemical uptake by plants from soil and the atmosphere," *Environmental Science and Technology* 28(13), 2259-2266.

Pelletier, O., Ritter, L., and Somers, C. J. (1989). "Disposition of 2,4-dichloro-phenoxyacetic acid dimethylamine by fischer 344 rats dosed orally and dermally," *J. Toxicol. Environ. Health* 28, 221-234.

Pennington, J. A. T. (1994). *Food value of portions commonly used*. 16th ed. J.B. Lippincott, Philadelphia, PA.

Perrin, D. D., Dempsey, B., and Serjeant, E. P. (1981). *pKa prediction for organic acids and bases*. Chapman and Hall, New York..

Perry, R. H., et al. (1997). *Perry's chemical engineer's handbook*, 7th ed., McGraw-Hill, New York.

Piper, W. N. (1973.) "Excretion and tissue distribution of 2,3,7,8 tetrachloro-dibenzo -p-dioxin in the rat," *Environ. Health Perspect.* 5, 241-244.

Potts, R. O., and Guy, R. H. (1992). "Predicting skin permeability," *Pharm. Res*. 9, 663-669.

Prinn, R., Cunnold, P., Simmonds, R., Alyea, R., Boldi, A., Crawford, P., Fraser, D., Gutzler, D., Hartley, R., Rosen, R., and Rasmussen R. (1992). "Global average concentration and trend for hydroxyl radicals deduced from ALE/GAGE trichloroethane (methyl chloroform) data for 1978-1990," *Journal of Geophysical Research* 97, 2445-61

Reeves, A. L. (1965)."The absorption of beryllium from the gastrointestinal tract," *Arch Environ. Health* 11, 209-214.

Reid, R. C., Prausnitz, J. M., and Sherwood, T. K. (1977). *The properties of gases and liquids*. 3rd ed., McGraw-Hill, New York, 544-601.

Riederer, M. (1995). "Partitioning and transport of organic chemicals between the atmospheric environment and leaves." *Plant contamination – Modeling and simulation of organic chemical processes.* S. Trapp and C. McFarlane, ed., Lewis, Boca Raton, FL, 153-190.

Reifenrath, W. G., et al. (2002). "Percutaneous absorption of explosives and related compounds: An empirical model of bioavailability of organic nitro compounds from soil," *Toxicol. Appl. Pharmacol.* 182, 160-168.

Rose, J. Q., Ramsey, J. C., Wentzler, T. H., Hummel, R. A., and Gehring, P. J. (1976). "The fate of 2,3,7,8 tetrachlorodibenzo-p-dioxin following single and repeated oral doses to the rat," *Toxicol. Appl. Pharmacol.* 36, 209-226.

Ruoff, W. (1995). "Relative bioavailability of manganese ingested in food or water." *Proceedings workshop on the bioavailability and oral toxicity of manganese.* USEPA-ECAO, Cincinnati, OH.

Sander, R. (1999). "Compilation of Henry's law constants for inorganic and organic species of potential importance in environmental chemistry," Ver 3, Max-Planck Institute for Chemistry, Air Chemistry Department, Mainz, Germany.

Sayato, Y., Nakamuro, K., Matsui, S., and Ando, M. (1980). "Metabolic fate of chromium compounds. I. Comparative behavior of chromium in rat administered with Na2 51 CrO4 and 51 CrCl3," *J. Pharm. Dyn.* 3, 17-23.

Sijm, D. T. H. M., and van der Linde, A. (1995). "Size-dependent bioconcentration kinetics of hydrophobic organic chemicals in fish based on diffusive mass transfer and allometric relationships," *Environmental Science and Technology* 29(11), 2769-77.

Strenge, D. L., Peterson, S. R., and Sager, S. (1989). "Chemical data bases for the multimedia environmental pollutant assessment system (MEPAS): Version 1," PNL-7145, Pacific Northwest Laboratory, Richland, WA.

Sweetman, A. J., Thomas, G. O., and Jones, K. C. (1999). "Modelling the fate and behaviour of lipophilic organic contaminants in lactating dairy cows," *Environ. Pollut*. 104, 261-270.

Tanabe, S. (1981). "Absorption efficiencies and biological half-life of individuals chlorobiphenyls in rats treated with kanechlor products," *Agric. Biol. Chem*. 45, 717-726.

Taylor, D. M., Bligh, P. H., and Duggan, M. H. (1962). "The absorption of calcium, strontium, barium, and radium from the gastrointestinal tract of the rat," *Biochem. J.* 83, 25-29.

Thacker, N. A., Prendergast, D., and Rockett, P. I. (1996). "B-fitting: A statistical estimation technique with automatic parameter selection." *Proceedings of the British Machine Vision Conference*, Edinburgh.

Thibodeaux, L. J. (1995). *Environmental chemodynamics: Movement of chemicals in air, water, and soil.* 2nd ed., Wiley, New York.

Thomann, R.V. (1989). "Bioaccumulation model of organic chemical distribution in aquatic food chains," *Environmental Science and Technology* 23(6), 699-707.

Thomann, R. V., Connolly, J. P., and Parkerton, T. F. (1992). "An equilibrium model of organic chemical accumulation in aquatic food webs with sediment interactions," *Environ. Tox. Chem*. 11, 615-629.

Thomas, G. O., Sweetman, A. J., and Jones, K. C. (1999). "Input-output balance of polychlorinated biphenyls in a long-term study of lactating dairy cows," *Environmental Science and Technology* 33(1), 104-112.

Thomas, G. O., Sweetman, A. J., Lohmann, R., and Jones, K. C. (1998). "Derivation and field testing of air-milk and feed-milk transfer factors for PCBs," *Environmental Science and Technology* 32(22), 3522-3528.

Trapp, S. (2000). "Modelling uptake into roots and subsequent translocation of neutral an ionisable organic compounds," *Pest-Management-Science* 56 (9), 767-778.

Trapp, S., and Matthies, M. (1995). "Generic one-compartment model for uptake of organic chemicals by foliar vegetation," *Environmental Science and Technology* 29(9), 2333-2338.

Trapp, S., Rasmussen, D., and Samsøe-Petersen, L. (2003). "Fruit tree model for uptake of organic compounds from soil," *SAR - QSAR Environ. Res.* 14, 17-26.

Travis, C. C., and Arms, A. D.. (1988). "Bioconcentration of organics in beef, milk, and vegetation," *Environmental Science and Technology* 22(3), 271-274.

Tunkel, J., Howard, P. H., Boethling, R. S., Stiteler, W., and Loonen, H. (2000). "Predicting ready biodegradability in the miti test," *Environ. Toxicol. Chem.* 19, 2478-2485.

United States Environmental Protection Agency. (1984)." Risk analysis of TCDD contaminated soil," EPA/600/8-84/031, Office of Health and Environmental Assessment, Exposure Assessment Group, Washington, DC. (NTIS, Springfield, VA; PB-85-145704.)

_____ . (1988). "Hospital waste combustion study: Data gathering phase," EPA-450/3-88-008, Office of Air Quality Planning and Standards, Research Triangle Park, NC.

United States Environmental Protection Agency. (1989). "Risk assessment guidance for superfund. Human health evaluation manual: Part A. Interim final," Office of Solid Waste and Emergency Response, Washington, DC. (NTIS PB-90-155581.)

_____ . (1992a). "Dermal exposure assessment: Principles and applications," Office of Health and Environmental Assessment, EPA/600/6-88/005Cc.

_____ . (1992b). "Technical support document for the land application of sewage sludge, Volumes I and II," EPA 822/R-93-001a, Office of Water. Washington, DC. (NTIS PB93-110575, ERIC = #D734).

_____ . (1994). "Air emissions models for waste and wastewater, WATER9," http://www.epa.gov/ttn/chief/software/water/

_____ . (1995a). "Great Lakes water quality initiative, Technical support document for the procedure to determine bioaccumulation factors," EPA-820-B-95-005, Office of Water.

_____ . (1995b). "Memorandum regarding further studies for modeling the indirect exposure impacts from combustor emissions," Environmental Criteria and Assessment Office, Washington, DC.

_____ . (1995c). "Review draft development of human health based and ecologically based exit criteria for the hazardous waste identification project," Volumes I and II, Office of Solid Waste.

_____ . (1995d). "Supplemental guidance to RAGS: Region 4 bulletins, Human health risk assessment (Interim Guidance)," Waste Management Division, Office of Health Assessment, http://www.epa.gov/region4/waste/ots/otsguid.htm.

_____ . (1995e). "OAQPS," Emission Factor and Inventory Group, Air Emission Models Wastewater Treatment, Version 4.0, Research Triangle Park, NC.

United States Environmental Protection Agency. (1996). "Soil screening guidance: Technical background document," EPA/540/R95/128, Office of Emergency and Remedial Response, Washington, DC. (NTIS PB96-963502.)

_____ . (1997a). "Food Ingestion Factors," *Exposure factors handbook*. Volume II. EPA/600/P-95/002Fb.

_____ . (1997b). "Health effects assessment summary tables," Office of Research and Development, Washington, DC.

_____ . (1998). "Screening level ecological risk assessment protocol for hazardous waste combustion facilities," Draft Interim Final. April.

_____ . (2000). "Integrated risk information (IRIS)," http://www.epa.gov/iriswebp/iris/intro.htm#ref ["What is IRIS?"] and http://www.epa.gov/iriswebp/iris/subst/index.html ["IRIS Substance List"].

_____ . (2001a). "List of contaminants & their MCLs," http://www.epa.gov/safewater/mcl.html#mcls.

_____ . (2001b). "EPA Region III RBC table," Region III, Washington, DC.

_____ . (2003). "Multimedia, multipathway, and multireceptor risk assessment (3MRA) modeling system, Volume II: Site-based, regional, and national data," EPA530-D-03-001b, Office of Research and Development, Athens, GA.

_____ . (2004a). Office of Superfund, Washington, DC. Online database: http://hhpprtv.ornl.gov/

_____ . (2004b). "Risk assessment guidance for Superfund, Volume I: Human health evaluation manual (Part E, Supplemental guidance for dermal risk assessment) final," EPA/540/R/99/005 OSWER 9285.7-02EP PB99-963312.

Vecchia, B. E. (1997). "Estimating the dermally absorbed dose from chemical exposure: Data analysis, parameter estimation, and sensitivity to parameter uncertainties," M.S. Thesis, Colorado School of Mines, Golden, CO.

Veith, G. D., Defoe, D. L., and Bergstedt, B .V. (1979). "Measuring and estimating the bioconcentration factor of chemicals in fish," *Journal Fisheries Research Board of Canada* 36, 1040-1048.

Veith, G. D., Macek, K. J., Petrocelli, S. R., and Carroll, J. (1980). "An evaluation of using partition coefficients and water solubility to estimate bioconcentration factors for organic chemicals in fish." *Aquatic toxicology*. J. G. Eaton, P. R. Parish, and A. C. Hendricks, ed., ASTM STP 707, American Society for Testing and Materials.

Waitz, J. A., Ober, R .E., Meisenhelder, J. E., and Thompson, P. E. (1965). "Physiological disposition of antimony after administration of 124 Sb-labeled tartar emetic to rats, mice and monkeys, and the effects of tris (p-aminophenyl) carbonium pamoate on this distribution," *Bull. World Health Organization* 33, 537-546.

Weast, R. C. (1981). *Handbook of chemistry and physics*. 62nd ed. CRC Press, Cleveland, OH.

Weininger, D. (1988). "SMILES, a chemical language and information system. 1. Introduction to methodology and encoding rules," *J. Chem. Inf. Comput. Sci.* 28, 31-36.

Wester, R. C., Maibach, H. I., Bucks, D. A. W., Sedik, L., Melendres, J., Laio, C. L., and DeZio, S. (1990). "Percutaneous absorption of [14C]DDT and [14C]Benzo(a)pyrene from soil," *Fund. Appl. Toxicol*. 15, 510-516.

Wester, R. C., Maibach, H. I., Sedik, L., Melendres, J., DeZio, S., and Wade, M. (1992a). "In-vitro percutaneous absorption of cadmium from water and soil into human skin, *Fund. Appl. Toxicol*. 19, 1-5.

Wester, R. C., Maibach, H. I., Sedik, L., Melendres, J., Laio, C. L., and DeZio, S. (1992b). "Percutaneous absorption of [14C]chlordane from soil," *J. Toxicol. Environ. Health* 35, 269-277.

Wester, R. C., Maibach, H. I., Sedik, L., Melendres, J., and Wade, M. (1993a). "In-vivo and in-vitro percutaneous absorption and skin decontamination of arsenic from water and soil." *Fund. Appl. Toxicol.* 20, 336-340.

_____ . (1993b). "Percutaneous absorption of PCBs from soil: In-vivo rhesus monkey, in-vitro human skin, and binding to powered human stratum corneum," *J. Toxicol. Environ. Health* 39, 375-382.

Wester, R. C., Maibach, H .I., Sedik, L., Melendres, J., Wade, M, and DeZio, S. (1993c). "Percutaneous absorption of pentachlorophenol from soil," *Fund. Appl. Toxicology* 20, 68-71.

Wester, R. C., Melendres, J., Logan, F., Hui, X., and Maibach, H. I. (1996). "Percutaneous absorption of 2,4-Dichlorophenoxyacetic acid from soil with respect to the soil load and skin contact time: In-vivo absorption in rhesus monkey and in vitro absorption in human skin," *J. Toxicol. Environ. Health* 47, 335-344.

Wilke, C. R., and Lee, C. Y. (1955). "Estimation of diffusion coefficients for gases and vapors," *Ind. Eng. Chem.* 47, 1253-1257.

Young, V. R., Nahapetian, A., and Janghorbani, M. (1982). "Selenium bioavailability with reference to human nutrition," *Am. J. Clin. Nutr*. 35, 1076-1088.

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

Appendix A
TOPKAT Quantitative Structural Activity Relationships System

The TOPKAT system (Accelrys, Inc., San Diego, CA) consists of a basic program that controls data entry, toxicity estimate calculations, and search functions for its model databases. An individual module is provided for each toxicologic endpoint, e.g., LD50, LOAEL, mutagenicity, carcinogenicity (male rat), carcinogenicity (female rat), etc.

A module may contain more than one database, each comprised of compounds in a certain structural class, e.g., multiple benzenes, alicyclics, etc. All predictive equations and validation procedures applied to a given query compound are based on the database for the structural class to which the query belongs. Thus, from each database a separate model is developed for making estimates of the relevant endpoint for chemicals in that structural class.

Each database contains a substantial number of compounds, often between 100 and 300, and an indication for each compound of the actual toxicity, carcinogenicity, etc., from laboratory data, and whether it was used in generating the model. If it was used in model generation, the toxicity prediction for the compound, generated by the model, is also given. Generally, a small number of compounds are omitted from model generation as outliers or as wielding an undue influence on the model. Typically the models yield an accuracy of about 95 percent for compounds in the model's database and compounds falling within the model's "optimum prediction space" (OPS).

The TOPKAT predicts the toxicity of a chemical structure based on statistically derived structure-activity relationships (SARs). The models are discrete molecular descriptors that identify functional groups present on a molecule and other parameters that can be used to quantify attributes of a particular structure. Standard databases were evaluated to obtain experimental values as input to the SAR equations.

For toxicity endpoints displaying continuous values, such as rat oral acute LD50 and rat chronic LOAEL, the system uses linear multiple regression equations and the predictions represent estimates in dose units (milligrams per kilogram). For dichotomous endpoints, such as carcinogenicity and Ames

mutagenicity, the models use two-group linear discriminate functions, and the output represents a probability, from 0 to 1, of a positive outcome for that endpoint. TOPKAT considers probability estimates form 0.3 to 0.7 to be indeterminate.

Carcinogenicity endpoints were estimated for four animal models (male rat, female rat, male mouse, and female mouse). Each TOPKAT predictive model is developed from its own separate database and is limited to one of the foregoing animal models. Each covers a wide range of organic compounds, both aliphatic and aromatic. Results for a given compound sometimes vary from one animal model to another, even when confidence in the estimate is high or moderate.

Probable responses in rabbit eye and skin irritation tests (Draize) estimate probability of a severe response, and also probability of a negative response. These two probabilities are then combined into an overall estimate, e.g., mild/moderate, severe, less than severe, or "not negative."

TOPKAT software includes an extensive procedure for internal validation of the estimate. The system checks to see if all substructures that comprise the query compound are represented among the compounds included in the database. The query compound is characterized by many descriptors, and the resulting multivariate description, or position in a multidimensional space, is automatically checked against the multidimensional OPS of the model. Generally, the SAR predictions generated by TOPKAT show a high probability of being accurate when all substructures are covered and the compound falls within the calculated OPS.

In all cases where actual data are not available, the user attempts to determine what level of confidence should be placed in the estimate. For estimates generated by the more recent versions of the software, the determinations provided by the built-in validation procedures are of first importance. Other factors used in developing suggestions of high, medium, or low confidence include, without being limited to:

- Whether all major structural features of the query compound are well represented in the model's database. (At a certain level this results in an automatic warning from the software.)
- Whether there are in the database a number of compounds that are judged by the software to be electrotopologically close to the query compound.
- Whether these nearby compounds are estimated accurately by the model and tend to present toxicity levels similar to that estimated for the query compound.
- Whether the model's database is reasonably large.
- Whether the compounds in the model's database are in general estimated with high accuracy.

For many estimates, meaningful results are not obtained. This usually results from the location of the query compound outside of the model's OPS, and not within an acceptable distance from the OPS, or, alternatively, the presence in the

query compound of a molecular fragment not adequately represented in the model's database.

For QSAR results, such as those discussed here, varying degrees of uncertainty always exist. It is common for about 80 to 90 percent of compounds not present in the pertinent database (but within the OPS of the model) to be predicted within a factor of five of the experimental value. Quantitative predictions, including mouse LC50, rat LD50, and rat chronic LOAEL, are accompanied by a 95 percent confidence range; these typically encompass values within a factor of four or five in either direction.

Appendix B
Table of Toxicity Benchmark Values

Table B1
Firing Range Compounds of Suspected Concern (Noncarcinogenic Values)

Substance	CAS Number	RfD_o		RfD_i		Comments
		mg/kg/day	Reference	mg/kg/day	Reference	
1,2-dichloroethene (cis)	156-59-2					
1,2-dichloroethene (trans)	156-60-5	2.00E-02	IRIS			
(1,2-dichloroethyl) benzene[1]	1074-11-9					Subchronic testing of noncancer toxicity recommended
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	1.40E-01	HEAST-Alt	
1,2-dichloro-3-methylbenzene[2]	32768-54-0	2.04E-02	CHPPM			Prov. RfD_o based on QSAR
1,2-dichloroethene (cis/trans mixture)	540-59-0	1.00E-02	HEAST			
1,3,5-trimethylbenzene (mesitylene)	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[2]	106-99-0	6.70E-02	CHPPM			Prov. RfD_o based on QSAR
1,3-dinitrobenzene	99-65-0	1.00E-04	IRIS			
1,4-diamino-2,3-dihydroanthraquinone (DDA) violet-dye mix[1]	81-63-0					Subchronic testing of noncancer toxicity recommended
1,4-di-p-toluidinoanthraquinone (PTA) solvent green 3[1]	128-80-3					Subchronic testing of noncancer toxicity recommended
1-butanol	71-36-3	1.00E-01	IRIS			
1-butene[2]	106-98-9	3.50E-02	CHPPM			Prov. RfD_o based on RfD_o estimate for related cpd. (IRIS)
1-chloro-2-methylbenzene	95-49-8	2.00E-02	IRIS			
1-chloro-3-methylbenzene[2]	108-41-8	6.70E-03	CHPPM			Prov. RfD_o based on published RfD_o for related cpd.
1-hexene[2]	592-41-6	1.02E-01	CHPPM			Prov. RfD_o based on QSAR
1-pentene[2]	109-67-1	3.50E-02	CHPPM			Prov. RfD_o based on RfD_o estimate for related cpd.
1-(methylamino)anthraquinone (disperse red 9)[1]	82-38-2	2.90E-02	CHPPM			Prov. RfD_o based on QSAR
2-(2-quinolyl)-1,3-indandione (D & C yellow no. 11) or (solvent yellow 33)	8003-22-3	4.00E-02	CHPPM			Prov. RfD_o based on est. of expt'l rodent subchron. LOAEL (TOXLINE)
2,3-butanedione	431-03-8	1.70E-01	CHPPM			Prov. RfD_o based on QSAR
2,3,7,8-tetrachlorodibenzo-p-dioxin	1746-01-6	n/a				Prov. RfD_o estimate not made/high cancer potential
2,4,6-trinitrotoluene (TNT)	118-96-7	5.00E-04	IRIS			

(Sheet 1 of 7)

[1] No value calculated - further research is recommended.
[2] Provisional value calculated - further research is recommended.

Table B1 (Continued)

Substance	CAS Number	RfD_o		RfD_i		Comments
		mg/kg/day	Reference	mg/kg/day	Reference	
2,4-dinitrotoluene (DNT; 2,4-DNT)	121-14-2	2.00E-03	IRIS			
2,6-dinitrotoluene (2,6-DNT)	606-20-2	1.00E-03	HEAST			
2,5-dimethylfuran[2]	625-86-5	1.60E-02	CHPPM			Prov. RfD_o based on QSAR
2-amino-4,6-dinitrotoluene	35572-78-2	6.00E-05	EPA-NCEA			
2-amino-9,10-anthracenedione (a) (AAQ)[2]	117-79-3	1.80E-01	CHPPM			Prov. RfD_o based on expt'l rat chronic LOAEL = 175 mg/kg/day (TOPKAT database)
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	HEAST-Alt	
2-heptanone[2]	110-43-0	1.70E-01	CHPPM			Prov. RfD_o based on QSAR
2-methyl-1-butene[2]	563-46-2	1.40E-01	CHPPM			Prov. RfD_o based on QSAR (Table 27)
2-methylfuran[2]	534-22-5	6.90E-03	CHPPM			Prov. RfD_o based on QSAR
2-methylthiophene[2]	554-14-3	1.70E-02	CHPPM			Prov. RfD_o based on QSAR
2-nitrotoluene (ONT)	88-72-2	1.00E-02	HEAST			
2-pentanone[2]	107-87-9	1.40E-01	CHPPM			Prov. RfD_o based on QSAR
2-propanol[2]	67-63-0	5.80E-02	CHPPM			Prov. RfD_o based on QSAR
2-thiophenecarboxaldehyde[2]	98-03-3	1.80E-02	CHPPM			Prov. RfD_o based on QSAR
3-(phenylhydrazone)-1H-indole-2,3-dione[2]	17310-26-8	4.00E-02	CHPPM			Prov. RfD_o based on QSAR
3-furaldehyde[2]	498-60-2	3.80E-03	CHPPM			Prov. RfD_o based on QSAR
3-methyl-1-butene[1]	563-45-1					Subchronic testing of non-cancer toxicity recommended
3-methylfuran[2]	930-27-8	2.10E-03	CHPPM			Prov. RfD_o based on QSAR of related cpd.
3-methylthiophene[2]	616-44-4	1.70E-02	CHPPM			Prov. RfD_o based on QSAR
3-nitrotoluene	99-08-1	1.00E-02	EPA-NCEA			
4-1,2,4-oxadizaolin-3-one-2,5-diphenyl-delta[1]	None found					Subchronic testing of non-cancer toxicity recommended
4-amino-2,6-dinitrotoluene (4ADNT)[2]	19406-51-0	5.00E-04	CHPPM			Prov. RfD_o based on published RfD_o for related cpd. (IRIS)
4-ethyltoluene[2]	622-96-8	5.50E-03	CHPPM			Prov. RfD_o based on QSAR
4-methyl-2-pentanone	108-10-1	8.00E-02	HEAST	2.00E-02	HEAST-Alt	
4-nitrotoluene	99-99-0	1.00E-02	HEAST			
4-phenoxy-2(1H)-quinolinone		1.30E-02	CHPPM			Prov. RfD_o based on QSAR
acenaphthene	83-32-9	6.00E-02	IRIS			
acenaphthylene[2]	208-96-8	9.10E-03	CHPPM			Prov. RfD_o based on QSAR
acetaldehyde	75-07-0			2.57E-03	IRIS	

(Sheet 2 of 7)

[1] No value calculated - further research is recommended.
[2] Provisional value calculated - further research is recommended.

Table B1 (Continued)

Substance	CAS Number	RfD_o		RfD_i		Comments
		mg/kg/day	Reference	mg/kg/day	Reference	
acetaldehyde	75-07-0			2.57E-03	IRIS	
acetic acid[2]	64-19-7	2.50E-02	CHPPM			Prov. RfD_o based on TLV (ACGIH)
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	n/a				Prov. RfD_o estimate not made/simple asphyxiant
Acrolein	107-02-8	2.00E-02	HEAST	5.7×10^{-6}	IRIS	
Acrylonitrile	107-13-1	3.00E-02	IRIS	5.7×10^{-4}	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			
Barium	7440-39-3	7.00E-02	IRIS	1.40E-04	HEAST-Alt	
benzaldehyde	100-52-7	1.00E-01	IRIS			
benzanthrone (b)[2]	82-05-3	5.90E-02	CHPPM			Prov. RfD_o based on QSAR
Benzene	71-43-2	3.00E-03	EPA-NCEA	1.70E-03	EPA-NCEA	
benzo(a)anthracene	56-55-3	n/a				Prov. RfD_o estimate not made/high cancer potential
benzo(a)pyrene	50-32-8	n/a				Prov. RfD_o estimate not made/high cancer potential
benzo(b)fluoranthene	205-99-2	n/a				Prov. RfD_o estimate not made/high cancer potential
benzo(e)pyrene[2]	192-97-2	1.20E-01	CHPPM			Prov. RfD_o based on QSAR
benzo(g,h,i)perylene[2]	191-24-2	4.20E-02	CHPPM			Prov. RfD_o based on QSAR
benzo(k)fluoranthene	207-08-9	n/a				Prov. RfD_o estimate not made/high cancer potential
benzofuran[2]	271-89-6	2.10E-02	CHPPM			Prov. RfD_o based on expt'l rat chronic LOAEL = 21.4 mg/kg/day (TOPKAT database)
benzonitrile[2]	100-47-0	1.70E-02	CHPPM			Prov. RfD_o based on QSAR
beryllium	7440-41-7	2.00E-03	IRIS	5.70E-06	IRIS	
bis(2-ethylhexyl)phthalate	117-81-7	2.00E-02	IRIS			
butanal[2]	123-72-8	7.30E-02	CHPPM			Prov. RfD_o based on QSAR
cadmium	7440-43-9	1.00E-03	IRIS	5.70E-05	EPA-NCEA	
calcium	7440-70-2	n/a				Considered essential nutrient/toxic potential low

(Sheet 3 of 7)

[1] No value calculated - further research is recommended.
[2] Provisional value calculated - further research is recommended.

Table B1 (Continued)

Substance	CAS Number	RfD_o		RfD_i		Comments
		mg/kg/day	Reference	mg/kg/day	Reference	
carbon dioxide (CO2)	124-38-9	n/a				Prov. RfD_o estimate not made/simple asphyxiant
carbon disulfide	75-15-0	1.00E-01	IRIS	2.00E-01	IRIS	
carbon monoxide (CO)	630-08-0	n/a				Prov. RfD_o estimate not made/asphyxiant
carbon tetrachloride	56-23-5	7.00E-04	IRIS	5.71E-04	EPA-NCEA	
carbonyl sulfide[1]	463-58-1					Subchronic testing of noncancer toxicity recommended
chlorobenzene	108-90-7	2.00E-02	IRIS	1.70E-02	EPA-NCEA	
chloroethene (vinyl chloride)	75-01-4	3.00E-03	IRIS	2.80E-02	IRIS	
chloroform	67-66-3	1.00E-02	IRIS	8.60E-05	EPA-NCEA	
chloromethane	74-87-3			8.60E-02	EPA-NCEA	
chromium	7440-47-3	3.00E-03	IRIS	3.00E-05	IRIS	
chrysene	218-01-9	n/a				Prov. RfD_o estimate not made/high cancer potential
cis-2-butene[2]	590-18-1	1.10E-01	CHPPM			Prov. RfD_o based on QSAR
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[2]	53-70-3	6.80E-02	CHPPM			Prov. RfD_o based on QSAR
dibenzo(b,def)chrysene-7,14 dione (c.i. vat yellow 4)[2]	128-66-5	3.50E-01	CHPPM			Prov. RfD_o based on expt'l rat chr LOAEL = 350 mg/kg/day (TOPKAT database)
dibutyl phthalate	84-74-2	1.00E-01	IRIS			
dichloroacetonitrile[2]	3018-12-0	8.00E-03	CHPPM			Prov. RfD_o based on expt'l rat subchr. NOAEL = 8 mg/kg/day (HSDB)
dichlorodiflouromethane	75-71-8	2.00E-01	IRIS	5.00E-02	HEAST-Alt	
Dimethyltrisulfide[1]	3658-80-8					Subchronic testing of noncancer toxicity recommended
diphenylamine	122-39-4	2.50E-02	IRIS			
ethane	74-84-0	n/a				Prov. RfD_o estimate not made/simple asphyxiant
ethanol	64-17-5	1.90E+00	CHPPM			Prov. RfD_o based on TLV (ACGIH)/relative toxicty low
ethyl benzene	100-41-4	1.00E-01	IRIS	2.90E-01	IRIS	
ethyl chloride	75-00-3			2.86E+00	IRIS	
ethylene	74-85-1	n/a				Prov. RfD_o estimate not made/simple asphyxiant
fluoranthene	206-44-0	4.00E-02	IRIS			

[1] No value calculated - further research is recommended.

[2] Provisional value calculated - further research is recommended.

Table B1 (Continued)

Substance	CAS Number	RfD_o		RfD_i		Comments
		mg/kg/day	Reference	mg/kg/day	Reference	
formaldehyde	50-00-0	2.00E-01	IRIS			
furan	110-00-9	1.00E-03	IRIS			
HCl	7647-01-0			5.70E-03	IRIS	
Heptanal[2]	111-71-7	1.20E-01	CHPPM			Prov. RfD_o based on QSAR
hexachlorobenzene	118-74-1	8.00E-04	IRIS			
hexachlorobutadiene	87-68-3	2.00E-04	HEAST			
hexachlorocyclopentadiene	77-47-4	6.00E-03	IRIS	2.00E-04	IRIS	
hexachloroethane	67-72-1	1.00E-03	IRIS			
Hexanal[2]	66-25-1	1.10E-01	CHPPM			Prov. RfD_o based on QSAR
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 (isobutane)[1]	75-28-5	4.90E-02	CHPPM			Prov. RfD_o based on QSAR of related cpd.
i-butene (isobutene/e-butylene)[1]	115-11-7	1.60E-01	CHPPM			Prov. RfD_o based on QSAR
indeno(1,2,3-cd)pyrene[1]	193-39-5					Subchronic testing of noncancer toxicity recommended
Isothiocyanatomethane[1]	556-61-6					Subchronic testing of noncancer toxicity recommended
lead	7439-92-1	n/a				Not needed/IEUBK model used to estimate risk
xylene (mixed isomers)	1330-20-7					
m-xylene (meta-xylene)	108-38-3	2.00E+00	IRIS			
p-xylene (para-xylene)	106-42-3	2.00E+00	IRIS			
magnesium	7439-95-4	n/a				Prov. RfD_o estimate not made/inorganic or metal/relatively low toxicity from oral route
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[1]	78-85-3	5.00E-04	CHPPM			Prov. RfD_o based on published RfD_o for related cpd. (IRIS)
methane	74-82-8	n/a				Prov. RfD_o estimate not made/simple asphyxiant
methylene chloride	75-09-2	6.00E-02	IRIS	8.60E-01	HEAST	
methylnitrite[1]	624-91-9					Subchronic testing of noncancer toxicity recommended

(Sheet 5 of 7)

[1] No value calculated - further research is recommended.
[2] Provisional value calculated - further research is recommended.

Table B1 (Continued)

Substance	CAS Number	RfD_o		RfD_i		Comments
		mg/kg/day	Reference	mg/kg/day	Reference	
methyl-t-butylether (MTBE)	1634-04-4			8.57E-01	IRIS	
methyl-vinyl ketone[2]	78-94-4	1.30E-04	CHPPM			Prov. RfD_o based on est.of expt'l subchron. LOAEL (abstr. In TOXLINE)
naphthalene	91-20-3	2.00E-02	IRIS	8.57E-04	IRIS	
n-butane[2]	106-97-8	6.00E-02	CHPPM			Prov. RfD_o based on published RfD_o for related cpd. (HEAST)
n-decane[2]	124-18-5	3.30E-01	CHPPM			Prov. RfD_o based on QSAR
NH3 (ammonia)	7664-41-7			2.86E-02	IRIS	
nickel	7440-02-0	2.00E-02	IRIS	(2.00E-03)	ATSDR	
nitric acid	7697-37-2	n/a				Prov. RfD_o estimate not made/inorganic or metal/acute irritant
nitrobenzene	98-95-3	5.00E-04	IRIS	6.00E-04	HEAST-Alt	
nitrogen oxide (NOx)	10024-97-2	1.00E+00	IRIS (w)			
Nitroglycerine[2]	55-63-0	1.70E-04	CHPPM			Prov. RfD_o based on clinical dose of 5.0 mg/kg/day (HSDB)
nitromethane[2]	75-52-5	1.40E-03	CHPPM			Prov. RfD_o based on QSAR
nonanal[2]	124-19-6	1.60E-01	CHPPM			Prov. RfD_o based on QSAR
OCDD (1,2,3,4,6,7,8,9-OCDD)	3268-87-9	n/a				Prov. RfD_o estimate not made/high cancer potential
octanal[2]	124-13-0	1.40E-01	CHPPM			Prov. RfD_o based on QSAR
o-dichlorobenzene	95-50-1	9.00E-02	IRIS			
o-methoxy-phenyl-azo-b-naphthol (oil red g)[1]	1229-55-6					Subchronic testing of noncancer toxicity recommended
o-xylene (ortho-xylene)	95-47-6	2.00E+00	IRIS			
particulate cyanide	57-12-5	2.00E-02	IRIS			
p-dichlorobenzene (para-dichlorobenzene)	106-46-7	3.00E-02	EPA-NCEA	2.29E-01	IRIS	
pentaerythritoltetranitrate (PETN)	78-11-5	n/a				Prov. RfD_o estimate not made; cpd is relatively nontoxic
perchloroethylene	127-18-4	1.00E-02	IRIS	1.40E-01	EPA-NCEA	
phenanthrene[2]	85-01-8	4.00E-02	CHPPM			Prov. RfD_o based on QSAR
phenol	108-95-2	6.00E-01	IRIS			
phenylacetylene (ethynyl benzene)[1]	536-74-3					Subchronic testing of noncancer toxicity recommended

(Sheet 6 of 7)

[1] No value calculated - further research is recommended.

[2] Provisional value calculated - further research is recommended.

Table B1 (Concluded)

Substance	CAS Number	RfD_o		RfD_i		Comments
		mg/kg/day	Reference	mg/kg/day	Reference	
phosphorus	7723-14-0	2.00E-05	IRIS			
propanal	123-38-6	5.50E-02	CHPPM			Prov. RfD_o based on QSAR
propane	74-98-6	6.00E-02	CHPPM			Prov. RfD_o based on published RfDo for related cpd. (HEAST)
propylene	115-07-1	n/a				Prov. RfD_o estimate not made/simple asphyxiant
propyne[2]	74-99-7	1.70E+00	CHPPM			Prov. RfD_o based on TLV (ACGIH)
pyrene	129-00-0	3.00E-02	IRIS			
RDX	121-82-4	3.00E-03	IRIS			
selenium	7782-49-2	5.00E-03	IRIS			
silver	7440-22-4	5.00E-03	IRIS			
styrene (vinyl benzene)	100-42-5	2.00E-01	IRIS	2.86E-01	IRIS	
sulfur dioxide (SO2)	7446-09-5	n/a				Prov. RfD_o estimate not made/acute irritant
sulfuric acid	64-67-5	n/a				Prov. RfD_o estimate not made/acute irritant
tetryl (2,4,6-trinitrophenylmethylnitramine)	479-45-8	1.00E-02	HEAST			
thallium	7440280	7.00E-05	Other (Reg III)			Prov. RfD_o estimate not made/inorganic or metal
thiophene[2]	110-02-1	1.50E-02	CHPPM			Prov. RfD_o based on QSAR
toluene	108-88-3	2.00E-01	IRIS	1.14E-01	IRIS	
trans-2-butenal[2]	123-73-9	6.10E-03	CHPPM			Prov. RfD_o based on QSAR
trans-2-butene[1]	624-64-6					Subchronic testing of noncancer toxicity recommended
trans-2-pentene[2]	646-04-8	8.50E-02	CHPPM			Prov. RfD_o based on QSAR
trans-3-penten-2-one[1]	3102-33-8					Subchronic testing of noncancer toxicity recommended
trichloroethylene (TCE)	79-01-6	6.00E-03	EPA-NCEA			
trichloroflouromethane	75-69-4	3.00E-01	IRIS	2.00E-01	HEAST-Alt	
vinylidenechloride	75-35-4	5.00E-02	IRIS			
zinc	7440-66-6	3.00E-01	IRIS			

(Sheet 7 of 7)

[1] No value calculated - further research is recommended.

[2] Provisional value calculated - further research is recommended.

Table B2
Firing Range Compounds of Suspected Concern (Carcinogenic Values)

Substance	CAS Number	CSF_o		CSF_i		Comments
		1/mg/kg/day	Reference	1/mg/kg/day	Reference	
1,2-dichloroethene (cis)	156-59-2					
1,2-dichloroethene (trans)	156-60-5					Negative in-vitro data. No testing suggested at this time
(1,2-dichloroethyl) benzene	1074-11-9					None. Insufficient information to determine suitability
1,2,4-trimethylbenzene	95-63-6					Negative in-vitro data. No testing suggested at this time
1,2-dichlorethane	107-06-2	9.10E-02	IRIS	7.40E-03	IRIS	
1,2-dichloro-3-methylbenzene	32768-54-0					None. Insufficient information to determine suitability
1,2-dichloroethene (cis/trans mixture)	540-59-0					Negative in-vitro data. No testing suggested at this time
1,3,5-trimethylbenzene (mesitylene)	108-67-8					Negative in-vitro data. No testing suggested at this time
1,3,5-trinitrobenzene	99-35-4					Positive in-vitro data; animal studies negative
1,3-butadiene	106-99-0			1.00E-01	IRIS	
1,3-dinitrobenzene	99-65-0					No further in-vitro testing/animal testing suggested
1,4-diamino-2,3-dihydroanthraquinone (DDA) violet-dye mix	81-63-0					Conflicting in-vitro data. Mechanistic evaluation recmd
1,4-di-p-toluidinoanthraquinone (PTA) solvent green 3	128-80-3					Conflicting in-vitro data. Mechanistic evaluation recmd
1-butanol	71-36-3					No further in-vitro testing/animal testing suggested
1-butene	106-98-9					None. Insufficient information to determine suitability
1-chloro-2-methylbenzene	95-49-8					Negative in-vitro data. No testing suggested at this time
1-chloro-3-methylbenzene	108-41-8					Negative in-vitro data. No testing suggested at this time
1-hexene	592-41-6					None. Insufficient information to determine suitability
1-pentene	109-67-1					None. Insufficient information to determine suitability

(Sheet 1 of 9)

Table B2 (Continued)

Substance	CAS Number	CSF_o		CSF_i		Comments
		1/mg/kg/day	Reference	1/mg/kg/day	Reference	
1-(methylamino)anthraquinone (disperse red 9)	82-38-2					None. Insufficient information to determine suitability
2-(2-quinolinyl)-1,3-indandione (D & C yellow no. 11) or (slovent yellow 33)	8003-22-3					Conflicting in-vitro data. Mechanistic evaluation recmd
2,3-butanedione	431-03-8					Positive in-vitro data; animal/mechanistic studies recmd
2,3,7,8-tetrachlorodibenzo-p-dioxin	1746-01-6	1.50E+05	HEAST	1.50E+05	HEAST	
2,4,6-trinitrotoluene (TNT)	118-96-7	3.00E-02	IRIS			
2,4-dinitrotoluene (DNT; 2,4-DNT)	121-14-2					Yes, animal studies for carcinogenicity mode/mechanism
2,6-dinitrotoluene (2,6-DNT)	606-20-2					Yes, animal studies for carcinogenicity mode/mechanism
2,5-dimethylfuran	625-86-5					Negative in-vitro data. No testing suggested at this time
2-amino-4,6-dinitrotoluene	35572-78-2					Conflicting in-vitro data. Mechanistic evaluation recmd
2-amino-9,10-anthracenedione (a) (AAQ)	117-79-3					No further in-vitro testing, but follow-up suggested
2-butanone	78-93-3					No further in-vitro testing suggested
2-furaldehyde	98-01-1					Yes. Currently insufficient and/or contradictory evidence
2-heptanone	110-43-0					Further in-vitro data needed; few data available
2-methyl-1-butene	563-46-2					None. Insufficient information to determine suitability
2-methylfuran	534-22-5					Negative in-vitro data. No testing suggested at this time
2-methylthiophene	554-14-3					Negative in-vitro data. No testing suggested at this time
2-nitrotoluene (ONT)	88-72-2	1.00E-02	HEAST			Negative in-vitro data. No testing suggested at this time
2-pentanone	107-87-9					None. Food additiive, GRAS, or under FDA oversight
2-propanol	67-63-0					No further in-vitro testing suggested

(Sheet 2 of 9)

Table B2 (Continued)

Substance	CAS Number	CSF_o		CSF_i		Comments
		1/mg/kg/day	Reference	1/mg/kg/day	Reference	
2-thiophenecarboxaldehyde	98-03-3					None. Insufficient information to determine suitability
3-(phenylhydrazone)-1H-indole-2,3-dione	17310-26-8					None. Insufficient information to determine suitability
3-furaldehyde	498-60-2					None. Insufficient information to determine suitability
3-methyl-1-butene	563-45-1					None. Insufficient information to determine suitability
3-methylfuran	930-27-8					Not recommended
3-methylthiophene	616-44-4					No information found, in-vitro screens recommended
3-nitrotoluene	99-08-1					No further in-vitro testing suggested
4-1,2,4-oxadizaolin-3-one-2,5-diphenyl-delta						No information found, in-vitro screens recommended
4-amino-2,6-dinitrotoluene (4ADNT)	19406-51-0					Conflicting in-vitro data. Mechanistic evaluation recmd
4-ethyltoluene	622-96-8					Negative in-vitro data. No testing suggested at this time
4-methyl-2-pentanone	108-10-1					No further in-vitro testing suggested
4-nitrotoluene	99-99-0	1.00E-02	HEAST			
4-phenoxy-2(1H)-quinolinone	6666-28-0					None. Insufficient information to determine suitability
acenaphthene	83-32-9					Negative in-vitro data. No testing suggested at this time
acenaphthylene	208-96-8					In-vitro testing advisable
acetaldehyde	75-07-0			6.29E-04	IRIS	
acetic acid	64-19-7					Negative in-vitro data. No testing suggested at this time
acetone	67-64-1					No further in-vitro testing suggested
acetonitrile	75-05-8	5.40E-01	IRIS			No further in-vitro testing suggested
acetophenone	98-86-2					No further in-vitro testing suggested

(Sheet 3 of 9)

Table B2 (Continued)

Substance	CAS Number	CSF_o 1/mg/kg/day	CSF_o Reference	CSF_i 1/mg/kg/day	CSF_i Reference	Comments
acetylene	74-86-2					None. Insufficient information to determine suitability
acrolein	107-02-8					No further in-vitro testing suggested
acrylonitrile	107-13-1	5.40E-01	IRIS	1.94E-02	IRIS	
aluminum	7429-90-5					Undetermined. Few data available
anthracene	120-12-7					No further in-vitro testing suggested
antimony	7440-36-0					None. Elements unsuited to in-vitro screening methods
arsenic	7440-38-2	1.43E-03	IRIS	1.23E+00	IRIS	
barium	7440-39-3					No further in-vitro testing suggested
benzaldehyde	100-52-7					Conflicting in-vitro data. Mechanistic evaluation recmd
benzanthrone (b)	82-05-3					Conflicting in-vitro data. Mechanistic evaluation recmd
benzene	71-43-2	5.50E-02	IRIS	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					No further in-vitro testing suggested
benzo(g,h,i)perylene	191-24-2					No further in-vitro testing suggested
benzo(k)fluoranthene	207-08-9	7.30E-02	EPA-NCEA	3.10E-02	EPA-NCEA	
benzofuran	271-89-6					Yes, animal studies for carcinogenicity mode/mechanism
benzonitrile	100-47-0					Negative in-vitro data. No testing suggested at this time
beryllium	7440-41-7			0.69E+00	IRIS	
bis(2-ethylhexyl)phthalate	117-81-7	1.40E-02	IRIS	1.40E-02	EPA-NCEA	
butanal	123-72-8					Equivocal data. Mechanistic evaluation may be needed
cadmium	7440-43-9			0.51E+00	IRIS	

Table B2 (Continued)

Substance	CAS Number	CSF_o		CSF_i		Comments
		1/mg/kg/day	Reference	1/mg/kg/day	Reference	
calcium	7440-70-2					None. Elements unsuited to in-vitro screening methods
carbon dioxide (CO2)	124-38-9					None. Insufficient information to determine suitability
carbon disulfide	75-15-0					Negative in-vitro data. No testing suggested at this time
carbon monoxide (CO)	630-08-0					None. Likely unsuited to in-vitro screening methods
carbon tetrachloride	56-23-5	.06E-04	IRIS	4.29E-03	IRIS	
carbonyl sulfide	463-58-1					None. Insufficient information to determine suitability
chlorobenzene	108-90-7					Yes. Currently insufficient and/or contradictory evidence
chloroethene (vinyl chloride)	75-01-4	1.50E+00	IRIS	1.26E-03	IRIS	
chloroform	67-66-3	6.10E-03	IRIS	6.57E-03	IRIS	
chloromethane	74-87-3	7.30E-03	HEAST	3.50E-03	EPA-NCEA	
chromium	7440-47-3			2.90E+02	IRIS	
chrysene	218-01-9	7.30E-03	EPA-NCEA	3.10E-03	EPA-NCEA	
cis-2-butene	590-18-1					None. Insufficient information to determine suitability
Cl2 (a)	7782-50-5					No further in-vitro testing suggested
cobalt	7440-48-4	1.00E+00	IRIS			
copper	7440-50-8					No further in-vitro testing suggested
dibenz(a,h)anthracene	53-70-3	7.30E+00	EPA-NCEA			
dibenzo(b,def)chrysene-7,14 dione (c.i. vat yellow 4)	128-66-5					No further in-vitro testing suggested
dibutyl phthalate	84-74-2					No further in-vitro testing suggested
dichloroacetonitrile	3018-12-0					No further testing suggested at this time
dichlorodiflouromethane	75-71-8					Further in-vitro data needed; few data available
dimethyltrisulfide	3658-80-8					None. Food additiive, GRAS, or under FDA oversight
diphenylamine	122-39-4					No further in-vitro testing suggested

Table B2 (Continued)

Substance	CAS Number	CSF_o 1/mg/kg/day	CSF_o Reference	CSF_i 1/mg/kg/day	CSF_i Reference	Comments
ethane	74-84-0					None. Insufficient information to determine suitability
ethanol	64-17-5					No further in-vitro testing suggested
ethyl benzene	100-41-4					No further testing suggested at this time
ethyl chloride	75-00-3					Equivocal animal/in-vitro resuts; no testing recommended
ethylene	74-85-1					No further in-vitro testing suggested
fluoranthene	206-44-0					No further in-vitro testing suggested
fluorene	86-73-7					No further in-vitro testing suggested
formaldehyde	50-00-0			3.70E-04	IRIS	
furan	110-00-9					Yes, animal studies for carcinogenicity mode/mechanism
HCl	7647-01-0					In-vitro testing may be advisable
heptanal	111-71-7					Negative in-vitro data. No testing suggested at this time
hexachlorobenzene	118-74-1	1.60E+00	IRIS	1.30E-01	IRIS	
hexachlorobutadiene	87-68-3	7.80E-02	IRIS	6.29E-03	IRIS	
hexachlorocyclopentadiene	77-47-4					Classified E - not likely a carcinogen
hexachloroethane	67-72-1	1.40E-02	IRIS	1.14E-03	IRIS	
hexanal	66-25-1					Contradictory in-vitro data. Mechanistic evaluation recmd
hexane	110-54-3					
HMX	2691-41-0					In-vitro testing advisable
hydrogen cyanide	74-90-8					None. Likely unsuited to in-vitro screening methods
i-butane (isobutane)	71-36-3					In-vitro tests plausible, but not recommended
i-butene (isobutene/e-butylene)	106-98-9					None. Simple asphyxiant
indeno(1,2,3-cd)pyrene	193-39-3					Yes, animal studies for carcinogenicity mode/mechanism
isothiocyanatomethane	556-61-6					Yes, animal studies for carcinogenicity mode/mechanism

Table B2 (Continued)

Substance	CAS Number	CSF_o		CSF_i		Comments
		1/mg/kg/day	Reference	1/mg/kg/day	Reference	
lead	7439-92-1					Yes, Insufficient evidence to support B2 classification
xylene (mixed isomers)	1330-20-7					
m-xylene (meta-xylene)	108-38-3					Negative in-vitro data. No testing suggested at this time
p-xylene (para-xylene)	106-42-3					No further in-vitro testing suggested
magnesium	7439-95-4					
manganese	7439-96-5					No further in-vitro testing suggested
m-dichlorobenzene	541-73-1					No further in-vitro testing suggested
mercury	7439-97-6					No further in-vitro testing suggested
methacrolein	78-85-3					Equivocal in-vitro data. Mechanistic evaluation recmd
methane	74-82-8					No further in-vitro testing suggested
methylene chloride	75-09-2	7.50E-03	IRIS	1.34E+00	IRIS	
methylnitrite	624-91-9					None. Food additiive, GRAS, or under FDA oversight
methyl-t-butylether (MTBE)	1634-04-4					Yes. Insufficient and/or contradictory exp. evidence
methyl-vinyl ketone	78-94-4					Conflicting in-vitro data. Mechanistic evaluation recmd
naphthalene	91-20-3					Conflicting in-vitro data. Mechanistic evaluation recmd
n-butane	106-97-8					Negative in-vitro data. No testing suggested at this time
n-decane	124-18-5					Negative in-vitro data. No testing suggested at this time
NH3 (ammonia)	7664-41-7					Negative in-vitro data. No testing suggested at this time
nickel	7440-02-0					Yes, animal studies for carcinogenicity mode/mechanism
nitric acid	7697-37-2					Further in-vitro data needed; few data available
nitrobenzene	98-95-3					
nitrogen oxide (NOx)	10024-97-2					No further in-vitro testing suggested

(Sheet 7 of 9)

Table B2 (Continued)

Substance	CAS Number	CSF_o 1/mg/kg/day	CSF_o Reference	CSF_i 1/mg/kg/day	CSF_i Reference	Comments
nitroglycerine	55-63-0					Conflicting in-vitro data. Mechanistic evaluation recmd
nitromethane	75-52-5					Yes, Insufficient evidence to support B2 classification.
nonanal	124-19-6					Conflicting in-vitro data. Mechanistic evaluation recmd
OCDD (1,2,3,4,6,7,8,9-OCDD)	3268-87-9	1.00E-02				
octanal	124-13-0					None. Food additiive, GRAS, or under FDA oversight
o-dichlorobenzene	95-50-1					No further in-vitro testing suggested
o-methoxy-phenyl-azo-b-naphthol (oil red g)						Conflicting in-vitro data. Mechanistic evaluation recmd
o-xylene (ortho-xylene)	95-47-6					No further in-vitro testing suggested
particulate cyanide	57-12-5					No further testing suggested at this time
p-dichlorobenzene (para-dichlorobenzene)	106-46-7	2.40E-02	HEAST	2.20E-02	EPA-NCEA	
pentaerythritoltetranitrate (PETN)	78-11-5					Negative in-vitro data. No testing suggested at this time
perchloroethylene	127-18-4	5.20E-02	EPA-NCEA	2.00E-03	EPA-NCEA	
phenanthrene	85-01-8					Yes, animal studies for carcinogenicity mode/mechanism
phenol	108-95-2					No further in-vitro testing suggested
phenylacetylene (ethynyl benzene)	536-74-3					None. Insufficient data to determine suitability
phosphorus	7723-14-0					In-vitro testing may be advisable
propanal	123-38-6					Conflicting in-vitro data. Mechanistic evaluation recmd
propane	74-98-6					None. Simple asphyxiant
propylene	115-07-1					No further in-vitro testing suggested
propyne	74-99-7					Conflicting in-vitro data. Mechanistic evaluation recmd
pyrene	129-00-0					No further in-vitro testing suggested

Table B2 (Concluded)

Substance	CAS Number	CSF_o		CSF_i		Comments
		1/mg/kg/day	Reference	1/mg/kg/day	Reference	
RDX	121-82-4	1.10E-01	IRIS			
selenium	7782-49-2					No further in-vitro testing suggested
silver	7440-22-4					No further testing suggested at this time
styrene (vinyl benzene)	100-42-5					Yes. Insufficient and/or contradictory evidence
sulfur dioxide (SO2)	7446-09-5					No further testing suggested at this time
sulfuric acid	64-67-5					Yes, at micro-level carcinogenicity mode/mechanism
tetryl (2,4,6-trinitrophenylmethylnitramine)	479-45-8					Positive in-vitro data; animal/mechanistic studies recmd
thallium	7440-28-0					None. Elements unsuited to in-vitro screening methods
thiophene	110-02-1					Negative in-vitro data. No testing suggested at this time
toluene	108-88-3					No further in-vitro testing suggested
trans-2-butenal	123-73-9	1.90E+00	HEAST			
trans-2-butene	624-64-6					None. Simple asphyxiant
trans-2-pentene	646-04-8					None. Simple asphyxiant
trans-3-penten-2-one	3102-33-8					None. Insufficient information to determine suitability
trichloroethylene (TCE)	79-01-6	1.10E-02	EPA-NCEA	6.00E-03	EPA-NCEA	
trichloroflouromethane	75-69-4					Negative in-vitro data. No testing suggested at this time
vinylidenechloride	75-35-4					Yes. Currently insufficient and/or contradictory evidence
zinc	7440-66-6					No further in-vitro testing suggested

(Sheet 9 of 9)

Appendix C
List of Abbreviations

ABS	Dermal absorption fraction
ACGIH	American Conference of Governmental Industrial Hygienists
AEC	U.S. Army Environmental Center
AME	Average model error
ARAMS	Adaptive Risk Assessment Modeling System
ASI	Analytical Services, Inc.
BAF	Bioaccumulation factor
BCF	Bioconcentration factor
BTF	Biotransfer factors
CAS	Chemical Abstract Service
CHPPM	U.S. Army Center for Health Promotion and Preventive Medicine
CSFs	Cancer slope factors
DW	Dry weight
EL	Environmental Laboratory
EPD	Effective prediction domain
EPI	Estimation Programs Interface
ERDC	U.S. Army Engineer Research and Development Center
FDA	U.S. Food and Drug Administration
FSG	Fuller, Schettler, and Giddings
FW	Fresh weight
GI ABS	GI absorption fraction
GRAS	Generally recognized as safe
GV	GaussView
HCCPD	Hexachlorocyclopeantadiene

HLCs	Henry's law constants
IARC	International Agency for Research on Cancer
IRIS	Integrated Risk Information System
LOAEL	lowest observed adverse effect level
MCI	Molecular connectivity index
MCLs	Maximum contaminant levels
MF	Modifying factor
MRLs	Minimum risk levels
MW	Molecular weight
NIST	National Institute of Standards and Technology
NOAEL	No observed adverse effect level
NTP	National Toxicology Program
OPS	Optimum prediction space
PAHs	Polycyclic aromatic hydrocarbons
PBT	Persistence Bioaccumulation Toxicity
PCBs	Polychlorinated biphenyls
PCDD	Polychlorinated dibenzo-p-dioxin
PCDF	Polychlorinated dibenzofuran
PETN	Pentaerythritol tetranitrate
PPRTVs	Provisional peer-reviewed toxicity values
QB	QSAR Builder
QSAR	Quantitative structure activity relationship
QSPR	Quantitative structure property relationship
RAIS	Risk Assessment Information System
RfC	Reference Concentration
RfD	Reference Dose
RfD_i	Inhalation, Reference Dose
RfD_o	Oral, Reference Dose
rmse	Root mean square error
SARs	Structure-activity relationships
SMILES	Simplified Molecular Input Line Entry Specification
TLV	Threshold Limit Value
UF	Uncertainty factor
USEPA	U.S. Environmental Protection Agency

WHO	World Health Organization

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)*	2. REPORT TYPE	3. DATES COVERED *(From - To)*
December 2005	Final report	

4. TITLE AND SUBTITLE

Data Gap Analysis and Database Expansion of Parameters for Munitions Constituents

5a. CONTRACT NUMBER

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)

Mark Dortch, Mansour Zakikhani, John Furey, Richard Meyer, Scott Fant, Jeffrey Gerald, Mohammad Qasim, Herb Fredrickson, Patricia Honea, Howard Bausum, Karen Walker, and Mark Johnson

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;
U.S. Army Center for Health Promotion and Preventive Medicine
5158 Blackhawk Road, Aberdeen Proving Ground, MD 21010-5403

8. PERFORMING ORGANIZATION REPORT NUMBER

ERDC/EL TR-05-16

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

U.S. Army Corps of Engineers
Washington, DC 20314-1000

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

14. ABSTRACT

Training and munitions firing activities at military ranges are operations vital to the readiness of the U.S. Army. These activities involve the use of pyrotechnic, explosive, and incendiary compounds. During an initial effort, the U.S. Army Engineer Research and Development Center (ERDC) and the U.S. Army Center for Health Promotion and Preventive Medicine (CHPPM) developed a Range Database for 188 chemicals of range interest specified by the U.S. Army Environmental Center. Significant gaps existed in the initial database, which included 11 priority physicochemical properties and human toxicological benchmarks. In recognition of the substantial remaining data gaps in the Range Database, this study was conducted by ERDC and CHPPM to expand the database for additional properties and human exposure parameters and to fill data gaps to the extent possible, even to include computational or estimation methods, if appropriate. The study effort was divided into five property/parameter categories: physicochemical properties for fate and transport, human exposure parameters, food transfer factors, environmental degradation rates and half-lives, and human toxicological benchmarks. The accuracy of estimation methods was evaluated. Recommendations are made for estimation methods and future research to address any remaining data gaps or to improve estimates. The data are being added to a relational database.

15. SUBJECT TERMS

Estimation methods
Human exposure parameters and factors
Human toxicological benchmarks
Military range constituent database
Physicochemical properties

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		185	