EPA
United States
Environmental Protection
Agency

EPA/600/R-08/021 | October 2008 | www.epa.gov/ord

Risk-Based Criteria to Support Validation of Detection Methods for Drinking Water and Air

Office of Research and Development
National Homeland Security Research Center

EPA/600/R-08/021
October 2008

Risk-Based Criteria to Support Validation of Detection Methods for Drinking Water and Air

Prepared by
Margaret MacDonell, Maryka Bhattacharyya, Molly Finster, Megan Williams,
Kurt Picel, Young-Soo Chang, and John Peterson
Environmental Science Division
U.S. Department of Energy Argonne National Laboratory

In collaboration with
Femi Adeshina *(Project Officer)* and Cynthia Sonich-Mullin *(Director)*
National Homeland Security Research Center
U.S. Environmental Protection Agency Office of Research and Development

Disclaimer

The U.S. Environmental Protection Agency through its Office of Research and Development funded and managed the research described here. It has been subjected to the Agency's review and has been approved for publication. Note that approval does not signify that the contents reflect the views of the Agency nor does it constitute endorsement.

Executive Summary

This report was prepared to support the validation of analytical methods for threat contaminants under the U.S. Environmental Protection Agency (EPA) National Homeland Security Research Center (NHSRC) program. It is designed to serve as a resource for certain applications of benchmark and fate information for homeland security threat contaminants.

The report identifies risk-based criteria from existing health benchmarks for drinking water and air for potential use as validation targets. The focus is on benchmarks for chronic public exposures. The priority sources are standard EPA concentration limits for drinking water and air, along with oral and inhalation toxicity values. Many contaminants identified as homeland security threats to drinking water or air would convert to other chemicals within minutes to hours of being released. For this reason, a fate analysis has been performed to identify potential transformation products and removal half-lives in air and water so appropriate forms can be targeted for detection over time.

The risk-based criteria presented in this report to frame method validation are expected to be lower than actual operational targets based on realistic exposures following a release. Note that many target criteria provided in this report are taken from available benchmarks without assessing the underlying toxicological details. That is, although the relevance of the chemical form and analogues are evaluated, the toxicological interpretations and extrapolations conducted by the authoring organizations are not. It is also important to emphasize that such targets in the current analysis are not health-based advisory levels to guide homeland security responses.

This integrated evaluation of chronic public benchmarks and contaminant fate has identified more than 200 risk-based criteria as method validation targets across numerous contaminants and fate products in drinking water and air combined. The gap in directly applicable values is considerable across the full set of threat contaminants, so preliminary indicators were developed from other well-documented benchmarks to serve as a starting point for validation efforts. By this approach, at least preliminary context is available for water or air, and sometimes both, for all chemicals on the NHSRC list that was provided for this evaluation. This means that a number of concentrations presented in this report represent indirect measures derived from related benchmarks or surrogate chemicals, as described within the many results tables provided in this report.

The main findings of this evaluation to identify risk-based method validation targets are as follows:

1. Chronic benchmarks provide a useful basis for some low risk-based targets for analytical methods. Directly applicable, contaminant-specific public benchmarks for drinking water and air are somewhat limited across the entire suite of contaminants. Coverage is complete for the 15 radionuclides and about half the chemicals.
2. This report provides benchmarks for surrogates or fate products, as well as route-related benchmarks. Food residue limits for several pesticides and safety levels for biological contaminants in foods contribute to further coverage. A risk-based chronic exposure concentration is available in at least one medium for a majority of the threat contaminants. This also applies to the direct benchmarks, with more targets available for water than for air.

3. A fate analysis is essential to understanding the identity and timing of relevant degradation products that would form in water and air, so validation targets can also be identified for those compounds posing legitimate concern.
4. For chemicals lacking chronic public benchmarks, workplace limits for long-term exposures can be considered for context, prioritizing those that are explicitly health-based.
5. For chemicals lacking both chronic public and occupational benchmarks, depending on the contaminant and data available, information from acute exposure guidelines (usually derived from a level of health effect) can be compared with other guides and relative toxicity information to develop bounding context for method validation.
6. Preliminary context is provided for method validation in at least one medium for all threat chemicals in the NHSRC list by integrating information on related benchmarks, relative toxicity, and fate. One step that can be taken to address benchmark gaps across media is to evaluate the toxicity data for these contaminants, including the data underlying existing benchmarks. In addition, benchmark estimates should be revised to include toxicity from dermal exposure when supportive data exist.
7. A key gap for fate information is the identification of radical oxidation products in air. Although half-lives have been measured or can be generally estimated, specific identities are often missing. This gap limits the determination of benchmarks for a number of specific fate products in air that might pose health concerns.
8. For toxicity gaps, no-observed-adverse-effect levels to support chronic benchmarks are lacking for a number of chemicals, as are quantitative considerations of sensitive subgroups within many existing benchmarks. To fill such gaps, downward adjustments can be applied to account for uncertainty.
9. This report provides information useful in streamlining and prioritizing method validation and health-based evaluations. Fate, relative toxicity, and method limits are considered.

In addition, the report identifies eight areas for future study.

In summary, health-based information provides a crucial foundation for validation of analytical methods. Gaps identified in this study can help frame research and development for analytical methods as well as related fate and toxicity analyses. Combining information on fate, benchmarks, toxicity, and analytical methods strengthens the validation effort as well as other ongoing health-related research within NHSRC.

Table of Contents

Figures

Text Boxes

Tables

Acronyms and Abbreviations

Below are acronyms and abbreviations not specific to individual chemicals. The subsequent list provides Chemical-Specific Notation. (Additional terms used in appendices are defined there.)

AAL	acceptable ambient level (States of New York and Rhode Island)
ACGIH	American Conference of Governmental Industrial Hygienists
AEGL	acute exposure guideline level (NAS NAC)
AEL	airborne exposure limit (CHPPM and CDC)
ANSI	American National Standards Institute
AREL	acute reference exposure level (Cal/EPA OEHHA)
AT	averaging time
atm	atmosphere(s)
ATSDR	Agency for Toxic Substances and Disease Registry (DHHS)
BW	body weight
C_i	concentration of chemical i
Cal/EPA	California Environmental Protection Agency
CAS RN	Chemical Abstracts Service Registry Number (American Chemical Society)
CDC	Centers for Disease Control and Prevention (DHHS)
CEGL	continuous exposure guidance level (DoD U.S. Navy and NAS)
CF	conversion factor
CHPPM	Center for Health Promotion and Preventive Medicine (DoD U.S. Army)
Ci	curie(s)
CLP	Contract Laboratory Program (EPA)
CREL	chronic reference exposure level, inhalation (Cal/EPA OEHHA)
CVAFS	cold vapor atomic fluorescence spectrometry
d	day(s)
DHHS	U.S. Department of Health and Human Services
DHS	U.S. Department of Homeland Security
DoD	U.S. Department of Defense
DOE	U.S. Department of Energy
DOWS	Department of Water Supply (Maui County, HI)
DWEL	drinking water equivalent level (EPA)
DWLOC	drinking water level of comparison (EPA)
DWUR	drinking water unit risk
EC	electron capture
ED	exposure duration
EF	exposure frequency
EML	Environmental Measurements Laboratory (DHS)
EMSL	Environmental Monitoring Systems Laboratory
EPA	U.S. Environmental Protection Agency
ERMA	Environmental Risk Management Authority (New Zealand)
FID	flame ionization detector
f	fiber(s)
FSANZ	Food Standards Australia New Zealand

g	gram(s)
GC	gas chromatography
GPL	general population limit (CHPPM and CDC)
HA	health advisory (EPA)
HPLC	high performance liquid chromatography
HQ	hazard quotient
hr	hour(s)
I_i	intake of chemical i
ICP	inductively coupled plasma
IO	inorganic
IR	intake rate (ingestion or inhalation)
IRED	interim reregistration eligibility decision (EPA)
IRIS	Integrated Risk Information System (EPA, electronic database)
ISO	International Standards Organization
IT	isomeric transition
IUR	inhalation unit risk
kg	kilogram(s)
KH	Henry's law constant
L	liter(s)
lbs	pounds
LOAEL	lowest observed adverse effect level
M	million (e.g., Mf/L for million fibers/liter)
m^3	cubic meter(s)
MAK	maximale arbeitsplatz konzentration (German occupational limit)
MCL	maximum contaminant level (EPA)
MD	multidetector detection
MDCH	Michigan Department of Community Health
MDL	method detection limit
MEG	military exposure guideline (CHPPM)
MeV	million electron volts
mg	milligram(s)
mg/kg-d	milligram(s) per kilogram per day
mg/L	milligram(s) per liter
min	minute(s)
mL	milliliter(s)
ML	minimum level (of quantitation)
mo	month(s)
MOE	margin of exposure
MRL	minimal risk level (ATSDR)
MResL	maximum residue limit (NZFSA)
MS	mass spectrometry
MW	molecular weight
NAAQS	National Ambient Air Quality Standard(s) (EPA)
NAC	National Advisory Committee (NAS, for AEGLs)
NAS	National Academy of Sciences
NCEA	National Center for Environmental Assessment (EPA)
NERL	National Exposure Research Laboratory (EPA)

NESHAPs	National Emission Standards for Hazardous Air Pollutants (EPA)
NHSRC	National Homeland Security Research Center (EPA)
NIOSH	National Institute for Occupational Safety and Health (DHHS)
nm	nanometer(s) (one-billionth meter)
NOAEL	no observed adverse effect level
NYSDEC	New York State Department of Environmental Conservation
NZFSA	New Zealand Food Safety Authority
OAQPS	Office of Air Quality Planning and Standards (EPA)
OEHHA	Office of Environmental Health Hazard Assessment (Cal/EPA)
OEL	occupational exposure limit
OPP	Office of Pesticide Programs (EPA)
OPPT	Office of Pollution Prevention and Toxics (EPA)
OPPTS	Office of Prevention, Pesticides, and Toxic Substances (EPA)
ORD	Office of Research and Development (EPA)
OSHA	Occupational Safety and Health Administration
PEL	permissible exposure limit (OSHA)
PCM	phase contrast microscopy
pH	negative logarithm of the hydrogen ion concentration (in solution)
pCi	picocurie(s)
PPRTV	provisional peer reviewed toxicity value (EPA)
PUF	polyurethane foam
QAP	Quality Assessment Program
RED	reregistration eligibility document (EPA)
REL	recommended exposure limit (NIOSH)
RfC	reference concentration
RfD	reference dose
SAM	Standardized Analytical Methods (report)
sec	second(s)
SF	slope factor
SF	spontaneous fission
SI	International System of Units
SM	standard method
SOW	statement of work
SVOCs	semivolatile organic compounds
SW	solid waste
TEL	tolerable exposure limit (NZERMA)
TEEL	temporary emergency exposure limit (DOE)
TEM	transmission electron micrsoscopy
TIC	toxic industrial chemical
TLV	threshold limit value (ACGIH)
TO	toxic organics
TS	thermospray
USDA	U.S. Department of Agriculture
UF	uncertainty factor
µg	microgram(s)
µg/L	microgram(s) per liter
$\mu g/m^3$	micrograms(s) per cubic meter

UR	unit risk
UV	ultraviolet
WIDHFS	Wisconsin Department of Health and Family Services
wk	week(s)
yr	year(s)

Chemical-Specific Notation

This chemical-specific list is offered as a resource for agent codes and basic chemical names and to indicate potential relationships among various threat chemicals and selected fate products (noted in italics). This information is intended to be illustrative, not inclusive. That is, not all terms defined in the text or tables are included here, nor are all fate relationships.

AC	hydrogen cyanide (chemical formula HCN)
ACH	alphachlorohydrin, or 3-chloro-1,2-propanediol
As	arsenic (component of fate products of arsine; lewisites-1,2; ethyldichloroarsine)
BTEX	benzene, toluene, ethylbenzene, xylene *(representative gasoline components)*
CK	cyanogen chloride *(can form from natural humics and cyanide with chloramine)*
Cl_2	chlorine gas
CN	cyanide (also used to refer to the tear gas form, acetophenone)
CO	carbon monoxide *(fate product of dichlorvos, HCN, phorate, carbon disulfide, others)*
CO_2	carbon dioxide *(fate product of chloropicrin, CK, HCN, PFIB, phosgene, others)*
COC	ether group (C-O-C)
CS	tear gas, 2-chlorobenzylidene malonitrile (note: tear gas form CN is acetophenone)
CVAA	2-chlorovinylarsonous acid *(fate product of lewisite-1)*
CX	phosgene oxime, or hydroxy carbonimidic dichloride
DESH	diisopropyl ethyl mercaptoamine *(fate product of VX)*
DIMP	1,2-diisopropyl methylphosphonate *(by-product of sarin synthesis)*
DMP	dimethyl phosphite *(fate product of TMP)*
DPD	n,n-diethyl-p-phenylene diamine
EA 2192	S-[2-(diisopropylamino)ethyl] methylphosphonothioate *(fate product of VX)*
ECH	epichlorohydrin
ED	ethyldichloroarsine
EEPA	*O*-ethyl ethylphosphonothioic acid *(fate product of VE)*
EMPA	*O*-ethyl methylphosphonic acid *(fate product of GE, VM, VX, Vx)*
EMPTA	*O*-ethyl methylphosphonothioic acid *(fate product of VX)*
ETO	ethylene oxide
F	fluoride *(for fate product information, see HF below)*
F_2	fluorine *(sometimes combined with soluble fluoride, for benchmarks)*
FM	titanium tetrachloride
FNA	fuming nitric acid
GA	tabun; *O*-ethyl *N,N*-dimethylphosphoramidocyanidate
GB	sarin; *O*-isopropyl methylphosphonofluoridate
GD	soman; *O*-pinacolyl methylphosphonofluoridate
GE	ethyl sarin; ethyl GB; *O*-isopropyl ethylphosphonofluoridate
GF	cyclosarin; cyclohexyl sarin; *O*-cyclohexyl methylphosphonofluoridate

H	sulfur mustard (undistilled HD); di-2 chloroethyl sulfide, bis(2-chloroethyl) sulfide
HAA	haloacetic acid *(includes dichloroacetic acid, fate product of dichlorvos)*
HCl	hydrochloric acid/hydrogen chloride *(fate product of chloropicrin, CK, ED, FM, lewisites-1/2, nitrogen mustard, others)*
HCN	hydrogen cyanide (agent AC) *(fate product of GA)*
HD	distilled sulfur mustard (same CAS number as sulfur mustard, H)
HF	hydrofluoric acid/hydrogen fluoride *(fate product of GB, GD, GE, GF, PFIB, others)*
Hg	mercury
HN-2	nitrogen mustard-2 (also NH-2), or bis(2-chloroethyl)methylamine
HOCl	hypochlorous acid *(chlorination residual often found in drinking water)*
HOCN	cyanic acid *(fate product of cyanogen chloride)*
H_3PO_4	phosphoric acid *(fate product of agents GA, RP, VG, and many pesticides)*
H_2S	hydrogen sulfide *(fate product of phorate)*
H_2SO_4	hydrogen sulfate, sulfuric acid *(fate product of phorate)*
HT	sulfur mustard-T mixture; mixture of sulfur mustard (see above) and T, which is bis[2-(2 chloroethylthio)ethyl] ether
IMPA	O-isopropyl methylphosphonic acid *(fate product of GB)*
L (L 1)	lewisite-1; dichloro(2-chlorovinyl)arsine; 2 chlorovinyldichloroarsine
L-2	lewisite-2; bis(2-chlorovinyl)chloroarsine
L-3	lewisite-3; tris(2 chlorovinyl)arsine
LO	lewisite oxide *(fate product of lewisite)*
MPA	methylphosphonic acid *(fate product of GB, GD, GE, GF, VM, VX, Vx)*
NaCN	sodium cyanide (representative cyanide salt)
NH-2	nitrogen mustard-2 (also HN-2); or bis(2-chloroethyl)methyl amine
NH_3	ammonia *(fate product of cyanogen chloride, HCN)*
NO	nitric (nitrogen) oxide (*fate product of chloropicrin, HCN, diesel, NO_2, others)*
NO_2	nitrogen dioxide, nitrite *(fate product of chloropicrin, cyanogen chloride, HCN)*
NO_3	nitrate (fate product of chloropicrin, cyanogen chloride, HCN)
O_3	ozone (fate product of chloropicrin)
OH	hydroxide, hydroxyl radical
p	para (e.g., p-nitrophenol, fate product of methyl parathion)
PAH(s)	polycyclic aromatic hydrocarbon(s)
PCB(s)	polychlorinated biphenyl(s)
PCP	phencyclidine (also referred to as angel dust)
PFIB	perfluoroisobutylene
PH_3	phosphine (fate product of red phosphorus)
PO_4	phosphate (for fate product information, see H_3PO_4 above)
PS	chloropicrin
PTFE	polytetrafluoroethylene (also referred to as Teflon)
RP	red phosphorous
SA	arsine
SEB	staphylococcal enterotoxin B
SO_4	sulfate

T2	trichothecene (mycotoxin)
TDG	thiodiglycol (fate product of sulfur mustards H/HD and HT)
TEPP	tetraethyl pyrophosphate
$TiCl_4$	titanium tetrachloride
TMP	trimethyl phosphite
VE	O-ethyl-S-[2-(diethylamino)ethyl] ethylphosphonothioate (also as “thiolate”)
VG	O,O-diethyl-S-[2-(diethylamino)ethyl] phosphorothioate (also as “thiolate”)
VM	O-ethyl-S [2-(diethylamino)ethyl] methylphosphonothioate (also “thiolate”)
VX	O-ethyl-S [2-(diisopropylamino)ethyl] methylphosphonothioate (also as “thiolate”)
Vx	O-ethyl-S-[2-(dimethylamino)ethyl] methylphosphonothioate (also as “thiolate”)
WP	white phosphorus (comprises up to 0.2% of RP, same CAS number)

Acknowledgements

The authors wish to express their deep appreciation to many colleagues who contributed to the development of this report, including Chandrika Moudgal, Alan Weinrich and Deborah McKean of EPA; and Shanna Collie, Andrew Davidson, Lynne Haroun, Kelley Swanberg, Jennifer Mattler, Kathleen Mettel, Camarie Perry, Allison Jenkins, Melissa Liu, Jerusha Sparks, and Shirley Williams-Scott of the Argonne team. Their inputs and insights have been invaluable.

1 Introduction

This report was prepared to support the validation of analytical methods for threat contaminants under the U.S. Environmental Protection Agency (EPA) National Homeland Security Research Center (NHSRC) program. Its purpose is to identify risk-based criteria from existing health benchmarks for drinking water and air for potential use as validation targets.

The focus is on benchmarks for chronic public exposures. The priority sources are standard EPA concentration limits for drinking water and air, along with oral and inhalation toxicity values.

Report Objectives (Box 1)
1. Identify health-based benchmarks for contaminants identified as potential chemical and radiological threats for use in defining potential target concentrations for validating analytical methods
2. Assess the fate and persistence of these threat contaminants to identify other chemicals that could form in water and air, and identify potential benchmarks for them

Many contaminants identified as homeland security threats to drinking water or air would convert to other chemicals within minutes to hours of being released. For this reason, a fate analysis has been performed to identify potential transformation products and removal half-lives in air and water so appropriate forms can be targeted for detection over time. The role of this analysis is reflected in Box 1.

The risk-based criteria presented in this report to frame method validation are expected to be lower than actual operational targets based on realistic exposures following a release. Note that many target criteria provided in this report are taken from available benchmarks without assessing the underlying toxicological details. That is, although the relevance of the chemical form and analogues are evaluated, the toxicological interpretations and extrapolations conducted by the authoring organizations are not.

It is also important to emphasize that such targets in the current analysis are not health-based advisory levels to guide homeland security responses.

This report is designed to serve as a resource for certain applications of benchmark and fate information for homeland security threat contaminants. It is organized as follows:

- Chapter 2 identifies the threat contaminants and exposure routes considered.
- Chapter 3 describes the evaluation process, including the approach for calculating target criteria from benchmarks given in other measures such as doses.
- Chapter 4 provides benchmark and criteria results for air and water in companion tables organized by contaminant set and medium; fate notes are given for two key sets.
- Chapter 5 summarizes results and discusses how they can be applied, considering target criteria, fate processes and products, relative toxicities, and benchmark coverage.
- Chapter 6 presents overall findings and next steps.
- Appendix A illustrates the general process for identifying risk-based criteria to help guide detection validation.

2 Contaminants and Exposure Routes Evaluated

To frame analytical method development efforts as part of NHSRC program planning, NHSRC identified more than 100 contaminants as possible threats. The list included toxic industrial chemicals, chemical warfare agents, and radionuclides. A related list to support the validation of analytical methods contained 23 chemicals, split between industrial toxics and agents. Method validation targets for this set were the driver for this report.

Threat Contaminants Reviewed (Box 2)

Contaminants	Source
chemicals: chemical warfare agents and toxic industrial chemicals	Method Validation priority list
more chemical agents	NHSRC list and the recent EPA report on standardized analytical methods (SAM)
more industrial chemicals	NHSRC list
radionuclides	NHSRC list and 2007 SAM report
remaining chemicals or groups (classes or mixtures)	SAM report

Standard health-based benchmarks address two main exposure routes: inhalation and ingestion. Where the value accounts for other exposures such as dermal absorption, those contributions are incorporated into the target concentrations presented here. Benchmarks were evaluated in phases for the contaminant sets shown in Box 2 and Table 1 (specific contaminants are listed in Table 2).

The Standardized Analytical Methods (SAM) document (EPA 2008) reviews analytical methods for chemicals (including nonspecific mixtures: asbestos, polychlorinated biphenyls [PCBs], and kerosene), plus general chemical groups, as well as radionuclides, pathogens, and biotoxins. The SAM (EPA 2008) was reviewed to identify any additional contaminants not already addressed as either a primary threat or associated fate product from the NHSRC list in order to assess benchmarks to support validation targets for them. This review identified additional candidates for assessment. Most chemicals in the SAM report are also on the NHSRC list, and many of the additional compounds are fate products (already assessed) or precursors or impurities of those chemicals. This commonality illustrates the integration of the specified program, with core threat contaminants and associated chemicals being addressed across complementary projects.

Regarding the general chemical groups, the SAM report is organized by method type, so in some instances only a basic category is indicated. These five groups are diesel range and gasoline range organic compounds, volatile and semivolatile organic compounds (SVOCs), and metals not otherwise specified. Each covers an extensive set of chemicals.

For example, gasoline range organics cover hundreds of hydrocarbons that include alkanes, alkenes, and aromatic compounds like benzene, toluene, ethylbenzene, and xylene (BTEX). These last four chemicals (BTEX) were selected to represent gasoline in this report, together with n-hexane. For diesel-range organic compounds, benchmarks found for diesel exhaust are given in this report. For the other three general groups, a number of specific chemicals within those categories are already being evaluated, so they are not addressed further.

Table 1 identifies the sets of primary contaminants for which relevant risk-based criteria were assessed; several are represented by indirect benchmarks. Additional chemicals beyond those listed were also assessed, as reflected in Table 2.

Table 1 **Contaminants With Risk-Based Criteria (Direct or Indirect)**[a]

23 Priority Chemicals (Detection Validation Priority List)	**14 Additional Chemical Agents** (NHSRC List and SAM report)	**18 Additional Industrial Chemicals** (NHSRC List)	**15 Radionuclides** (NHSRC List and SAM report)
Chloropicrin	Arsine (SA)	Aldicarb (Temik)	Americium-241
Dichlorvos	Cyanogen chloride (CK)	Boron trichloride	Californium-252
Dicrotophos (Bidrin)	Cyclohexyl sarin (GF)	Boron trifluoride	Cesium-137
Dimethyl phosphite (DMP)	Ethyl sarin (GE)	Bromadiolone	Cobalt-60
Ethyldichloroarsine (ED)	Hydrogen cyanide (HCN, agent AC)	Cadmium	Curium-244
Fenamiphos	Mustard, nitrogen (HN-2/NH-2)	Carbofuran	Europium-154
Lewisite (L-1)	Perfluoroisobutylene (PFIB)	Carbon disulfide	Iridium-192
Lewisite 2 (L-2)	Red phosphorus (RP)	Chlorine	Plutonium-238
Lewisite 3 (L-3)	Tear gas (CS)	Cyanide salts as sodium cyanide	Plutonium-239
Methyl parathion	Titanium tetrachloride (FM)	Ethylene oxide (Oxirane)	Polonium-210
Mevinphos (Phosdrin)	VE	Fluorine	Radium-226
Mustard, sulfur (H)	VG	Furan	Ruthenium-103
Mustard, sulfur, distilled (HD, distilled H)	VM	Mercuric chloride	Ruthenium-106
Mustard, sulfur with T (HT)	Vx	Nitric acid (fuming)	Strontium-90
Nicotine		Oxamyl (Vydate)	Uranium-238
Phorate (Thimet)		Paraquat	**16 Additional Industrial Chemicals** (SAM report)
Sarin (GB)		Sodium fluoroacetate (fluoroacetate salt)	
Soman (GD)	*This set includes several chemical warfare agents from the earlier, larger NHSRC list that are also in the SAM report. Similarly, agents CS, FM, GE, PFIB, RP, VE, VG and VM are also on the larger NHSRC list as well as in the SAM report. Vx was included as a V-series nerve agent, and nitrogen mustard was included for similarity to the H agents.* *Two others from the earlier NHSRC list, phosgene oxime (agent CX) and Teflon (polyterafluoroethylene or PTFE), are not in the SAM report, so they were not evaluated further in this report.* *(Note that some agents such as HCN also have industrial applications; VG has also been used as a pesticide, while the pesticide chloropicrin was formerly agent PS.)*	Sulfur dioxide	Allyl alcohol
Strychnine		*Some primary contaminants on the NHSRC list are also fate products of chemicals already covered as priority compounds or additional chemical agents.* *These include ammonia; arsenic; formaldehyde; hydrogen chloride, fluoride, and sulfide; nitric acid and nitrogen dioxide; phosgene, phosphine; and hydrogen sulfate/sulfuric acid.* *Benchmarks for those chemicals are identified within the tables for the first two contaminant sets, so they are not repeated as main chemicals within this set.*	Asbestos
Tabun (GA)			1,2-Dichloroethane (ethylene dichloride)
Tetraethyl pyrophosphate (TEPP)			Diesel engine exhaust
Trimethyl phosphite (TMP)			1,2-Diisopropyl methylphosphonate (DIMP)
VX			1,4-Dithiane (diethylene disulfide)
			Gasoline range organics: see 5 noted below
			Kerosene
			Methyl isocyanate
			Phenol
			Polychlorinated biphenyls (PCBs)
			Propylene oxide
			Gasoline is represented by benzene, toluene, ethylbenzene, xylenes, and n-hexane. *Two above are linked to chemical agents: DIMP is a by-product of GB synthesis and 1,4-dithiane is linked to munitions production and storage and thermal degradation of sulfur mustards.*

[a] For chemical agents (in blue) indicators values for ED and nitrogen mustard represent fate products. For toxic industrial chemicals (in purple), the TEPP is represented by a fate product; remaining additional industrial chemicals from the SAM report not already accounted for by the NHSRC list or its key fate products are also provided. Chronic occupational levels exist for many of these and other chemicals for which no public benchmarks were found. Information is available to frame method validation across all chemical and radiological contaminants from NHSRC and SAM sets.

Table 2 Tables of Contaminant-Specific Information[a]

Table	Focus	Medium	Contaminants Evaluated
Report Body			
5	Criteria for public	Air (inhalation)	23 initial priorities in air plus many fate products
6	Criteria for public	Air (inhalation)	14 remaining agents in air plus many fate products
7	Criteria for public	Drinking water (oral)	23 initial priorities in water plus many fate products
8	Criteria for public	Drinking water (oral)	14 remaining agents in water plus many fate products
9	Criteria for public	Both air and drinking water	more industrial chemicals
10	Properties, decay products	Both air and drinking water	15 radionuclides plus radioactive progeny
11	Criteria for public	Both air and drinking water	15 radionuclides
12	Criteria for public	Both air and drinking water	threat contaminants and products combined

[a] Yellow indicates the table is for air, blue indicates water, and green indicates both. Shading for contaminant type matches that used in Table 2.

Threat contaminants are those on the NHSRC list or in the Standardized Analytical Methods (SAM) report (EPA 2007a), and they are considered the primary contaminants for this study. (These are distinguished from fate products not specifically identified in the SAM report or NHSRC list.)

Fate notes are included in the basic results table for priority compounds and additional chemical agents (Tables 5–8) because these groups are evaluated first as a main foundation for this report. Additional fate information highlighted in Chapter 5 (Table 13) covers these and most of the other chemicals.

3 Methodology

This section describes the overall evaluation process and specific calculations used to identify target criteria in air and water for method validation. The process is discussed in Section 3.1, and calculational details are presented in Section 3.2.

3.1 Evaluation Process

Three steps were involved in identifying the Risk-Based Criteria for validation targets:

1. Assess the fate and persistence of the threat contaminants to identify others likely to form if the parent were released to air or water, considering various transformation processes.
2. Identify concentration benchmarks relevant to the general public for these contaminants.
3. Identify dose benchmarks and derive concentrations.

These steps are illustrated in Appendix A, and key available benchmarks are listed in Table 3. More details for several drinking water benchmarks are provided in Appendix A.

Table 3 **Key Types of Concentration and Dose Benchmarks for Air and Drinking Water**[a]

Medium	Orgzn.	Benchmark	Application
Air	EPA	RfC: reference concentration (noncancer) IUR: inhalation unit risk (cancer)	General public, repeat-chronic exposures
Air	EPA	NAAQS: national ambient air quality standard	General public, repeat-chronic exposures
Air	EPA	PPRTV: provisional peer-reviewed toxicity value	General public, repeat-chronic exposures
Air	CDC	AEL GPL: airborne exposure limit, general population limit	General public for 24/7, multiple consecutive years
Air	ATSDR	MRL: minimal risk level	General public, acute, intermediate, chronic
Air	Cal/EPA	CREL: chronic reference exposure level	General public, repeat-chronic exposures
Air	NAS-NAC	AEGL: acute exposure guideline level	General public, single exposures up to 8 hr (for emergency response)
Water	EPA	RfD: reference dose (noncancer); SF, (unit risk) UR: slope factor; drinking water (DW) UR	General public, repeat-chronic exposures
Water	EPA	PPRTV: provisional peer-reviewed toxicity value	General public, repeat-chronic exposures
Water	EPA	MCL: maximum contaminant level	General public, repeat-chronic exposures
Water	EPA	HA: health advisory (lifetime; also 10 day [d], 1 d)	General public, repeat-chronic exposures
Water	EPA	DWEL: drinking water equivalent level	General public, repeat-chronic exposures
Water	ATSDR	MRL: minimal risk level	Military personnel, can be intake-adjusted
Water	CHPPM	MEG: military exposure guideline	Military personnel, can be intake-adjusted (from 5 or 15 L/d to 2 L/d) for relevance to public
Water	ERMA	TEL: tolerable exposure limit	General public, repeat-chronic exposures

[a] ASTDR = Agency for Toxic Substances and Disease Registry, within CDC; Cal/EPA = California EPA; CDC = Centers for Disease Control and Prevention; CHPPM = U.S. Army Center for Health Promotion and Preventive Medicine; ERMA = New Zealand Environmental Risk Management Authority; NAS-NAC = National Academy of Sciences-National Advisory Committee (for AEGLs). Other limits evaluated include the Navy and NAS continuous exposure guidance levels (CEGLs) for adults in submarines for 90 days.

Key available benchmarks are listed in Table 3.

The toxicity values were assessed according to the recommended EPA (2003a) hierarchy:

1. EPA Integrated Risk Information System (IRIS) values *(These toxicity values exist for a number of chemicals and routes, as a primary source for air and water benchmarks.)*
2. EPA provisional peer-reviewed toxicity values (PPRTVs) *(For direct chronic benchmarks, no unique values were found in the initial review.)*
3. All other values, including from regional, state, and international sources.

When multiple benchmarks are found, other values are also provided to offer further context. The emphasis is on EPA benchmarks that reflect the most recent analyses.

3.2 Calculational Approach

The approach for calculating target concentrations from established toxicity values is described in this section. The objective is to ensure transparency for the risk-based values presented in the report, so the calculations can be readily followed. For benchmarks given as doses rather than concentrations, the process involves combining an estimate of the intake or dose from the assumed repeat exposures over an extended time with an estimate of the associated toxicity for that chemical by the given route of exposure, such as ingestion of drinking water.

The intake for an individual can be calculated using the following equation (from EPA 1989):

$$I_i = \frac{C_i \times IR \times EF \times ED}{BW \times AT} \qquad \textit{(may apply a CF, where needed to adjust mass units)}$$

where:

I_i = intake of chemical *i* milligram(s) per kilogram per day (mg/kg-d)
C_i = concentration of chemical *i* in water microgram(s) per liter (µg/L) or air microgram(s) per cubic meter (µg/m^3)
IR = intake (ingestion or inhalation) rate, assumed to be 2 L water/d, or 20 cubic meters (m^3) air/d
EF = exposure frequency, assumed to be 365 d/yr
ED = exposure duration, assumed to be 30 yr
BW = body weight kilogram (kg), assumed to be 70 kg (adult)
AT = averaging time (in d): 10,950 d for noncancer effects; 25,550 d for cancer risk
CF = conversion factor, as indicated for a given calculation (e.g., 10^3 microgram per milligram [µg/mg])

(Note that exposure time is included with intake rate.) An ED of 30 years was used because it is generally assumed for contaminated sites.

The intake is combined with a route-specific toxicity value (e.g., from EPA IRIS or a PPRTV, or another source such as a dose value developed for the U.S. Army) to assess the potential for a noncancer effect or the probability of incurring cancer over a lifetime as a result of that exposure. Certain chemicals are considered to cause both cancer and noncancer effects, and toxicity can be indicated for oral or inhalation exposure or both. As determined from these toxicity data, chemical- and route-specific values have been developed to assess potential effects from these exposures.

$$\text{Noncancer hazard quotient (HQ)} = \frac{\text{Intake}}{\text{Reference dose}}\text{, or I/RfD.}$$

The potential for noncancer or cancer effects is evaluated by combining the toxicity value with the estimated intake, as follows (EPA 1989):

Cancer risk = Intake × Slope factor, or I × SF.

Intakes were initially estimated for both oral and inhalation exposures, such that these equations applied to both routes. However, inhalation toxicity values are now expressed as concentrations (e.g., mg or µg per m^3 air). The reference concentration (RfC) represents the target for noncancer effects, and the IUR level corresponding to an incremental risk of 10^{-6} is the target for the cancer endpoint in this analysis. Thus, the equations shown above are applied directly for oral exposures, and they also frame inhalation estimates, as indicated below.

Only oral and inhalation exposures are specifically evaluated in this report; consideration of other routes (such as dermal absorption) has been incorporated into some existing benchmarks, and, where indicated, those additional contributions would be reflected in future values, following a detailed review of relevant toxicity data. As a note, this calculation process was needed for only a limited number of chemicals because criteria could be determined directly from benchmark values for most. Toxicity values are applied as follows to identify the Risk-Based Criteria for detection validation:

To derive a target criteria for water from an oral RfD (mg/kg-d):

1. Multiply the RfD by 70 kg.
2. Divide by 2 L/d.
3. To convert milligrams per liter (mg/L) to µg/L, multiply by 1,000.

To derive a target water criteria from an oral SF (risk per mg/kg-d), for a 10^{-6} risk level:

1. Multiply 10^{-6} (the target risk level) by 70 kg and 25,550 d.
2. Divide by SF, 2 L/d, 365 d/yr, and 30 yr. *(Where a risk-specific concentration is given for a 10^{-6} risk, that level is used directly.)*
3. To convert mg/L to µg/L, multiply by 1,000.

To convert an RfC or reference concentration to an RfD, if desired:

1. Divide by 70 kg.
2. Multiply by 20 m^3/d.

For a number of contaminants, no chronic public benchmark was found, but various OELs exist. Those limits are not included in the main body of the report for two reasons. First, they apply to a different target group with exposure conditions that differ from those being assessed, i.e., typically for adults working 8 or 10 hours a day with evening and weekend recovery periods (although, for example, the Navy CEGLs are for continuous exposures over 3 months in a submarine). Second, although some aim to be strictly health-based (such as the threshold limit values [TLVs] of the American Conference of Governmental Industrial Hygienists [ACGIH]), many are not. That is, implementation factors including feasibility are also considered for various Occupational Safety and Health Administration (OSHA) permissible exposure limits (PELs) and National Institute for Occupational Safety and Health (NIOSH) recommended exposure limits (RELs). For example, feasibility is identified as a factor for the asbestos, formaldehyde, and ethylene oxide RELs.

Additional benchmarks and other data were pursued when a chronic public benchmark was not found so that preliminary context for method validation could be provided for all the chemicals, and radionuclides from the NHSRC list and SAM report. Thus, various OELs are presented which may suggest possible high bounds for validation. These include guidelines developed for chemical agents by the U.S. Army (CHPPM) to support deployed troops. Some of those values are based on the same studies used to define chronic public benchmarks, notably in drinking water. The drinking water values presented in Table 2 based on the CHPPM concentrations for deployed force intakes of 5 L/d are scaled to 2 L/d for the general public.

4

Results

Target criteria for the detection program determined from benchmarks relevant to the general public are presented in several tables in this section. Results are organized by chemical category and medium, as illustrated in Table 4. (Several fate products are common across chemicals and media, and the set of unique fate products within a table is indicated in parentheses.)

Table 4 **Contaminants Represented in Air and Drinking Water**

Table	Contaminants Assessed	With Related Benchmarks *(including for a fate product or surrogate)*		Risk-Based Chronic Exposure Criteria
		Primary Contaminants	Fate Products	Identified
Air				
Table 5	23 priority chemicals	14	54	68
Table 6	14 remaining agents	8	15	23
Table 9	34 more industrials	24	1 *(unique)*	25
Table 11	15 radionuclides	15	22	15
Total	*86 primary*	*61 in air*	92	131
Water				
Table 7	23 priority chemicals	20	53	73
Table 8	14 additional agents	5	16	21
Table 9	34 more industrials	32	2	34
Table 11	15 radionuclides	15	22	15
Total	*86 primary*	*72 in water*	93	143

[a] Several concentrations are from indirect benchmarks. Fate product subtotals include unique entries within media. To illustrate, dimethyl phosphite is both a primary contaminant and fate product in Tables 5 and 7, and hydrogen fluoride is a fate product in both Tables 7 and 8, as one of several products associated with more than one primary chemical. Table 12 includes more than 200 unique values covering approximately 100 chemical and radiological contaminants in air and water combined.

These results reflect an extensive review of contaminants separately identified on the NHSRC list and in the SAM report (2007a), and unique fate products identified for these contaminants in drinking water and air. The contaminants are addressed in five groups:

1. Initial priority list for method validation, split between industrial chemicals and agents
2. Remaining agents on the NHSRC list
3. Remaining toxic industrial chemicals on the NHSRC list
4. All radionuclides on the NHSRC list and in the SAM report

5. Remaining industrial chemicals and groups in the SAM report

The overview analysis of physical-chemical fate for the contaminants in the NHSRC list and SAM report identified hundreds of transformation products. Many are common to multiple parents, e.g., hydrogen fluoride and arsenic are fate products of several chemical warfare agents. Also, because moist air promotes hydrolysis, hydrolysis products may be found in both drinking water and air.

Risk-based validation targets for the initial priority chemicals and the rest of the chemical agents in air and water are presented in four companion tables in the main body of this report:

- Table 5 – priority chemicals and key products in air
- Table 6 – 14 additional agents and key products in air
- Table 7 – 23 priorities and products in drinking water
- Table 8 – 14 agents plus products in drinking water

Fate notes are included in these tables. Persistence indicators for air and water are represented by physical-chemical half-lives, organized according to the intervals shown in Box 3.

Shading for Persistence as Represented by Physical-Chemical Half-Life (Box 3)

Indicator	***Half-Life***
Short	Seconds–hours
Moderate	Days–weeks
Long	Weeks–months
Very long	Months–years

The risk-based targets for the rest of the chemicals are presented in:

- Table 9 – remaining industrial chemicals in water and air

Several fate products are included in this table, and associated highlights are given in Chapter 5. Unlike Tables 5–8, where fate products with benchmarks are italicized and indented beneath the parents, this combined media table is alphabetized, with parents listed in parentheses following the fate products. Where no directly applicable benchmark was found, parentheses are also used to indicate values conservatively represented by analogues or surrogates that are more toxic. Those values are offered as indicators so that a preliminary context can be provided for all primary contaminants, to help frame priorities for follow-on evaluations.

Table 5 Risk-Based Criteria for the Initial Priority Chemicals and Their Key Transformation Products in Air

Chemical	CAS RN	Air Concn. *(μg/m³)*	Basis	Citation/Link for Risk-Based Value	Fate Notes
Chloropicrin	76-06-2	0.4	CREL (Cal/EPA)	Cal/EPA 2005a *(Noncancer Chronic Reference Exposure Levels)*, http://www.oehha.org./air/chronic_rels/pdf/allchrels.pdf; this value was established in 2001 and is also summarized in Cal/EPA 2005b, http://www.arb.ca.gov/toxics/healthval/contable.pdf	Photolysis half-life is 18 hr to 20 d in simulated sunlight; forms phosgene and nitrosyl chloride, with rapid photolysis (3–4 min) to atomic chlorine and nitric oxide (NO); these free radicals form (O_3), (NO_2), and chlorinated hydrocarbons
Phosgene	*75-44-5*	*0.3*	RfC, 0.0003 mg/m³ (EPA IRIS)	EPA *(2006f)*, http://www.epa.gov/iris/subst/0487.htm; this was also identified as the earlier draft Cal/EPA CREL *(1997)* in EPA 2000a, http://www.epa.gov/ttn/atw/hlthef/phosgene.html	Intermediate photolysis product, with no direct photolysis at >290 nanometer (nm); atmospheric half-life estimates are 20 to 44 to >100 yr
Hydrogen chloride (HCl)	*7647-01-0*	*20*	RfC, 0.02 mg/m³ (EPA IRIS)	EPA *(1995a)*, http://www.epa.gov/iris/subst/0396.htm; non-EPA value is lower, the CREL 9 μg/m³ *(2000)* in Cal/EPA 2005a, http://www.oehha.ca.gov/air/chronic_rels/pdf/7647010.pdf	Hydrolysis product, is incorporated into moisture in air, subject to wet/dry deposition
Ozone (O_3)	*10028-15-6*	*160*	NAAQS, 0.08 ppm (EPA Office of Air Quality Planning and Standards [OAQPS])	EPA 1997b, http://www.epa.gov/air/criteria.html *(from 1997)* is 8-hr average; CREL *(from 1992)* is 180 micrograms/m³, Cal/EPA 2005b, http://www.arb.ca.gov/toxics/healthval/contable.pdf	Photolysis product of intermediate nitrosyl chloride; half-life is 7 to 30 minutes (min)
Nitrogen dioxide (NO_2)	*10102-44-0*	*100*	NAAQS (EPA OAQPS)	EPA 1997b, http://www.epa.gov/air/criteria.html; note that the air quality standard *(from 1990)* is the annual arithmetic mean; the CREL is 470 μg/m³ *(from 1992)*, in Cal/EPA 2005b, http://www.arb.ca.gov/toxics/healthval/contable.pdf	Rapidly interconverts with nitric oxide (NO) in sunlight; can then form nitrous and nitric acids in moist air
Nitric acid (HNO_3)	*7697-37-2*	*(86)* *(acute only)*	acute reference exposure level (AREL) (Cal/EPA)	Cal/EPA *(2000)*, only for *acute*, no chronic level found, http://www.oehha.org/air/acute_rels/allAcRELs.html	Forms from NO_2 in moist air; subject to wet/dry depositioin
Dichlorvos	62-73-7	0.5	RfC (EPA IRIS)	EPA *(1994)*, http://www.epa.gov/iris/subst/0151.htm; also the 1997 MRL; and see EPA 2000a (OPPTS no observed adverse effect level (NOAEL) and uncertainty factor [UF] chronic), IRIS identifies "study NOAEL of 0.05 mg/m³"— which with 10x interspecies and intraspecies factors results in a RfC of 0.5 μg/m³	Atmospheric half-life is 13.6 hr; hydroxyl radical half-life is 2 d, main products are phosgene and carbon monoxide (CO)
Phosgene	*75-44-5*	*0.3*	RfC, 0.0003 mg/m³ (EPA/IRIS)	EPA *(2006f)*, http://www.epa.gov/iris/subst/0487.htm; this was also identified as the 1997 draft Cal/EPA CREL in EPA 2000e, http://www.epa.gov/ttn/atw/hlthef/phosgene.html	See entry under chloropicrin; atmospheric half-life estimates extend from 20 to >100 yr
Carbon monoxide (CO)	*630-08-0*	*10,000*	NAAQS for CO (EPA OAPQS)	EPA 1997b, http://www.epa.gov/air/criteria.html; note that this standard *(from 1990)* is an 8-hr average annual ceiling value	Can persist for several weeks, can oxidize to CO_2

Table 5 Risk-Based Criteria for the Initial Priority Chemicals and Their Key Transformation Products in Air

Chemical	CAS RN	Air Concn *(µg/m^3)*	Basis	Citation/Link for Risk-Based Value	Fate Notes
Dicrotophos	141-66-2	Not available (oral and dermal toxicant)	Lowest observed adverse effect level (LOAEL) of 0.02 mg/kg-d, MOE target 300 (EPA OPPTS) (Table 3)	IRIS entry (11/01/1989) indicates "no data" for RfC estimation; IRIS considers RfC "not available." EPA 2006f and EPA 2006g (lowest observed adverse effect level [LOAEL]-margin of exposure [MOE] for long-term inhalation; note that the dose for the *intermediate* inhalation duration is 0.04 mg/kg-d), http://www.epa.gov/oppsrrd1/REDs/dicrotophos_ired_pdf, the LOAEL-MOE for 70-kg adult, 20 m^3/d gives 0.2µg/m^3	Hydroxyl radical oxidation half-life is estimated at 7.3 hr
Dimethylamine	*124-40-3*	*2*	Early CREL (Cal/EPA); DMA not currently (2005) listed as CREL	RfC withdrawn 01/01/1999 and is not available; early CREL, Cal/EPA *(2000)*, http://www.oehha.ca.gov/risk/pdf/APENDX-B.pdf	Hydrolysis product in moist air; the hydroxyl radical half-life is 6 hr, faster in polluted air
Methanol	*67-56-1*	*4,000*	CREL (Cal/EPA)	Cal/EPA 2005a (current list; this CREL established in 2000), http://www.oehha.ca.gov/air/chronic_rels/pdf/67561.pdf	Hydrolysis product, can form in moist air; hydroxyl radical half-life is 3–30 d
Phosphoric Acid	*7664-38-2*	*10*	RfC, 0.01 mg/m^3 (EPA/IRIS)	RfC, 0.01 mg/m^3 from EPA/IRIS, EPA *(1995)*, http://www.epa.gov/irish/subst/0697.htm; CREL is 7 microgram/m^3 from Cal/EPA 2005b, http://www.arb.ca.gov/toxics/healthval/contable.pdf	Can form in moist air; can persist as terminal fate product
Dimethyl phosphite (DMP or DMHP)	868-85-9	420	est. RfC, route-extrapolated from est. RfD (NAS-NRC)	NAS 2000a (provisional RfC from estimated RfD of 0.12 mg/kg-d), http://books.nap.edu/catalog.php?record_id= 9841, reflects conservative assumptions until more data are available	Can hydrolyze to phosphorous acid and methanol in moist air; hydrolysis half-life is 10–19 d
Methanol	*67-56-1*	*4,000*	CREL (Cal/EPA)	Cal/EPA 2005a (current list; this CREL established in 2000), http://www.oehha.ca.gov/air/chronic_rels/pdf/67561.pdf	Hydrolysis product, can form in moist air; hydroxyl radical half-life is 3–30 d
Phosphoric Acid	*7664-38-2*	*10*	RfC, 0.01 mg/m^3 (EPA/IRIS)	RfC, 0.01 mg/m^3 from EPA/IRIS, EPA *(1995)*, http://www.epa.gov/irish/subst/0697.htm; CREL is 7 microgram/m^3 from Cal/EPA 2005b, http://www.arb.ca.gov/toxics/healthval/contable.pdf	Can form in moist air; can persist as terminal fate product
Ethyldichloroarsine (agent ED)	598-14-1	*No specific air benchmark found for general public. Toxicity estimates for ED are available for military populations (EC50 for odor threshold of 1 mg/m^3 for 1 min exposure duration; incapacitating effects can occur at 5 mg/m^3 for 1 min; Table II-41, p. II-60) in the following report: Army, Marine Corps, Navy, Air Force (2005). Potential Military Chemical/Biological Agents and Compounds. FM 3-11.9. Commandant, US Army Chemical School, Ft. Leonard Wood, MO. (Approved for public release, distribution is unlimited); this entry is included to introduce fate products for which benchmarks exist*			Can hydrolyze in moist air to ethylarsenous oxide and HCI
Hydrogen chloride (HCl)	*7647-01-0*	*20*	RfC, 0.02 mg/m^3 (EPA IRIS)	EPA *(1995a)*, http://www.epa.gov/iris/subst/0396.htm; non-EPA value is lower, CREL 9 µg/m^3 (2000) in Cal/EPA 2005a, http://www.oehha.ca.gov/air/chronic_rels/pdf/arsenics.pdf	Primary hydrolysis product in moist air; subject to wet/dry deposition
Arsenic, inorganic	*7440-38-2*	*0.0002*	Estimated air concentration resulting in 1 x 10^{-6} risk; IUR at 0.0043 per µg/m^3, (EPA, IRIS)	No RfC established by EPA; EPA *(1998)*, http://www.epa.gov/iris/subst/0278.htm; CREL 0.03 µg/m^3 *(listed in 2001, study in 2000)*, Cal/EPA 2005b, http://www.oehha.ca.gov/air/chronic_rels/pdf/arsenics.pdf	Terminal product, atmospheric lifetime could be 5 to 15 d with loss due to deposition

Table 5 Risk-Based Criteria for the Initial Priority Chemicals and Their Key Transformation Products in Air

Chemical	CAS RN	Air Concn *(μg/m³)*	Basis	Citation/Link for Risk-Based Value	Fate Notes
Fenamiphos	22224-92-6	(1.4)	NOAEL of 0.061 mg/kg-d and MOE of 150 (turf applicators) (EPA OPPTS)	EPA/IRIS considers that there are no data to support an RfC; EPA 2002b (highest MOE for turf, common application type; note inhalation LOAEL is 0.85 mg/kg-d and inhalation NOAEL is 0.061 mg/kg-d), http://www.epa.gov/oppsrrd1/REDs/fenamiphos_ired.pdf identifies this inhalation NOAEL and MOE for short term and *intermediate* inhalation, translates to 1.4 μg/m³ for a 70-kg adult inhaling 20 m³/d	Hydroxyl radical oxidation half-life is 2 to 5 hr; forms the sulfoxide and sulfone
Fenamiphos sulfoxide	*31972-43-7*	*(1.4)*	Conservatively represented by derivation from NOAEL and MOE for parent indicator compound Fenamiphos (EPA OPPTS)	EPA 2002b (as above; sulfoxide is considered less toxic), http://www.epa.gov/oppsrrd1/REDs/fenamiphos_ired.pdf inhalation NOAEL and MOE for *intermediate* inhalation for parent suggest > 1.4 μg/m³ for this form, for a 70-kg adult, 20 m³/d	Primary oxidation product; subject to wet/dry deposition
Fenamiphos sulfone	*31972-44-8*	*(1.4)*	Conservatively represented by derivation from NOAEL and MOE for parent indicator fenamiphos (EPA OPPTS)	EPA 2002b (as above; sulfone is considered less toxic), http://www.epa.gov/oppsrrd1/REDs/fenamiphos_ired.pdf inhalation NOAEL and MOE for *intermediate* inhalation for parent suggest > 1.4 μg/m³ for this form, for a 70-kg adult, 20 m³/d	Forms from oxidation of the sulfoxide; subject to wet/dry deposition
Phosphoric Acid	*7664-38-2*	*10*	RfC, 0.01 mg/m³ (EPA/IRIS)	RfC, 0.01 mg/m³ from EPA/IRIS, EPA *(1995)*, http://www.epa.gov/irish/subst/0697.htm; CREL is 7 microgram/m³ from Cal/EPA 2005b, http://www.arb.ca.gov/toxics/healthval/contable.pdf	Can form in moist air; can persist as terminal fate product
Lewisite (Lewisite-1, agent L-1)	541-25-3	3	GPL of 0.003 mg/m³ for 7/24 exposure over years from assumed continuous source GPL (CDC)	CDC 1988 *(Final Recommendations for Protecting the Health and Safety against Potential Adverse Effects of Long-Term Exposure to Low Doses of Agents GA, GB, VX, Mustard Agent [H, HD, T] and Lewisite [L])*, http://wonder.cdc.gov/wonder/PrevGuid/p0000027/p0000027.asp	Can persist 1–3 d; in moist air, can hydrolyze rapidly (<2 min half-life) to CVAA (2-chlorovinylarsonous acid) and HCl; hydroxyl radical oxidation half-life about 1.2 d; ultraviolet absorption spectrum of 200–350 nm indicates some photodegradation may occur
2-Chlorovinylarsonous acid (CVAA)	*85090-33-1*	*(0.11)*	Estimated inhalation RfC derived from estimated RfD for L-1	Estimated RfC for CVAA developed from estimated RfD for Lewisite (finalized in Opresko et. al. 2001); see USACHPPM (1999) for calculation of est. RfC for CVAA	Primary hydrolysis product, can rapidly form in moist air within minutes; subject to wet/dry deposition
Lewisite oxide	*3088-37-7*	*(0.11)*	Estimated inhalation RfC derived from estimated RfD for L-1	Estimated RfC for Lewisite oxide developed from estimated RfD for Lewisite (finalized in Opresko et. al. 2001); see USACHPPM (1999) for calculation of est. RfC for Lewsite oxide and Watson and Dolislager (2007) for recent documentation.	Dehydration product of 2-chlorovinylarsonous acid; subject to wet/dry deposition

Table 5 Risk-Based Criteria for the Initial Priority Chemicals and Their Key Transformation Products in Air

Chemical	CAS RN	Air Concn. *($\mu g/m^3$)*	Basis	Citation/Link for Risk-Based Value	Fate Notes
Hydrogen chloride (HCl)	*7647-01-0*	*20*	RfC, 0.02 mg/m^3 (EPA IRIS)	EPA *(1995a)*, http://www.epa.gov/iris/subst/0396.htm; non-EPA value is lower, CREL 9 $\mu g/m^3$ *(2000)* in Cal/EPA 2005a, http://www.oehha.ca.gov/air/chronic_rels/pdf/7647010.pdf	Hydrolysis product, is incorporated into moisture in air; subject to wet/dry deposition
Arsenic, inorganic	*7440-38-2*	*0.0002*	Estimated air concentration resulting in 1 x 10^{-6} risk; IUR at 0.0043 per $\mu g/m^3$, (EPA IRIS)	No RfC established by EPA; EPA *(1998)*, http://www.epa.gov/iris/subst/0278.htm; CREL is 0.03 $\mu g/m^3$ *(listed in 2001, study in 2000)*, Cal/EPA 2005a, http://www.oehha.ca.gov/air/chronic_rels/pdf/arsenics.pdf	Terminal product, atmospheric lifetime could be 5 to 15 d with loss due to deposition
Lewisite (Lewisite-2, agent L-2)	40334-69-8	(3)	Conservatively represented by GPL for L-1 CDC 1988	CDC 1988 (as for L-1) (separate value not established for L-2 but is considered much less toxic than L-1	Can hydrolyze in moist air to bis(2-chlorovinyl)arsenious acid and HCl
Hydrogen chloride (HCl)	*7647-01-0*	*20*	RfC, 0.02 mg/m^3 (EPA IRIS)	EPA *(1995)*, http://www.epa.gov/iris/subst/0396.htm; non-EPA value is lower, CREL 9 $\mu g/m^3$ (2000) in Cal/EPA 2005a, http://www.oehha.ca.gov/air/chronic_rels/pdf/7647010.pdf	Hydrolysis product, is incorporated into moisture in air, subject to wet/dry deposition
Arsenic, inorganic	*7440-38-2*	*0.0002*	Estimated air concentration resulting in 1 x 10^{-6} risk ; IUR at 0.0043 per $\mu g/m^3$, (EPA IRIS)	No RfC established by EPA; EPA *(1998)*, http://www.epa.gov/iris/subst/0278.htm; CREL 0.03 $\mu g/m^3$ *(listed in 2001, study in 2000)*, Cal/EPA 2005a, http://www.oehha.ca.gov/air/chronic_rels/pdf/arsenics.pdf	Terminal product, atmospheric lifetime could be 5 to 15 d with loss due to deposition
Lewisite (Lewisite-3, agent L-3)	40334-70-1	(3)	Conservatively represented by GPL for L-1 (CDC, 1988)	CDC 1988 (as for L-1) (separate values not established for L-3 but is much less toxic than L-1	Resists hydrolysis; subject to wet/dry deposition
Methyl parathion	298-00-0	0.01	RfC, 0.01 to 0.08 $\mu g/m^3$ for seasonal and chronic exposures as calculated by CA Dept. of Pesticide Regulation in 1999 (Cal/EPA)	EPA/IRIS considers there to be no data to support a RfC; Cal/EPA 1999 *(Scientific Review Panel, Methyl Parathion)*, http://www.arb.ca.gov/srp/srp3.pdf ("the RfCs of methyl parathion calculated in the report…ranges from 0.01 -0.08 microgram/m^3…for seasonal and chronic exposures"); the lowest value of 0.01 microgram/m^3 is considered protective	Hydroxyl radical half-life is 6.5 hr to 3.6 d; could hydrolyze in moist air to p-nitrophenol and dimethylphosphorothioic acid with a half-life of 4–89 d
p-Nitrophenol	*100-02-7*	*0.1*	Proposed Rhode Island (2004) and NY acceptable ambient level (AAL), annual limit (New York Statement Department of Environmental Conservation [NYSDEC] and State of Rhode Island)	Proposed state acceptable ambient level, AAL, for New York State and Rhode Island (2004), http://www.dem.ri.gov/programs/benviron/air/pdf/airtoxgl.pdf. The Rhode Island MQ (minimal quantity) of 11 is in units of pounds/year (lbs/yr) and refers to the allowable facility emissions, not ambient air concentrations. For documentation, please see Rhode Island Air Toxics Guideline *(2004)* cited for *4-nitrophenol.*	Can form in moist air; hydroxyl radical half-life is 4 d; photolysis half-life can range from hr to >1 week (wk)

Table 5 Risk-Based Criteria for the Initial Priority Chemicals and Their Key Transformation Products in Air

Chemical	CAS RN	Air Concn. *(μg/m³)*	Basis	Citation/Link for Risk-Based Value	Fate Notes
Methyl paraoxon	*950-35-6*	*(0.01)*	Equivalent to calculated RfC for parent methyl parathion, 0.01 microgram/m³, as per Cal/EPA guidance (Cal/EPA)	Cal/EPA 1999 *(Scientific Review Panel, Methyl Parathion)*, http://www.arb.ca.gov/srp/srp3.pdf; considered methyl paraoxon potentially 10 times more toxic than parent by inhalation; nevertheless, Cal/EPA determined that "the calculation of reference concentration [for methyl parathion] takes into account the concomitant presence of methyl paraoxon at approximately 25% of the level of methyl parathion" (pp. 7-8, item 31 of Cal/EPA 1999).	Produced by oxygen radical oxidation; can hydrolyze to para-nitrophenol (above) and dimethylphosphoric acid, and the two compounds below
Methanol	*67-56-1*	*4,000*	CREL (Cal/EPA)	Cal/EPA 2005a *(current list; this CREL established in 2000)*, http://www.oehha.ca.gov/air/chronic_rels/pdf/67561.pdf	Hydrolysis product, can form in moist air; hydroxyl radical oxidation half-life is 3–30 d
Phosphoric acid	*7664-38-2*	*10*	RfC, 0.01 mg/m³ (EPA/IRIS)	RfC, 0.01 mg/m³ from EPA/IRIS, EPA *(1995)*, http://www.epa.gov/irish/subst/0697.htm; CREL is 7 microgram/m³ from Cal/EPA 2005b, http://www.arb.ca.gov/toxics/healthval/contable.pdf	Can form in moist air; can persist as terminal fate product
Mustard, sulfur (agent H) and distilled sulfur mustard (agent HD)	505-60-2	0.02	GPL (CDC, ATSDR)	CDC 2004 *(Interim Recommendations for Airborne Exposure Limits for Chemical Warfare Agents H and HD [Sulfur Mustard])*, http://www.cdc.gov/nceh/demil/files/Federal%20Register%20Mustard%20AEL%205_2004.pdf; this is also the intermediate MRL for sulfur mustard from 2003, in ATSDR 2005, http://www.atsdr.cdc.gov/mrls/index.htm	As for HD (pure version of H, is the distilled form), oxidizes to sulfoxide and then (in more oxidizing conditions) sulfone; estimated half-life for hydroxyl radical oxidation is 1.4 d, and atmospheric half-life is 2.1 d
Mustard sulfoxide	*5819-08-9*	*(0.02)*	Protectively represented by the H/HD value above (CDC, ATSDR)	CDC 2004 (as above for H), http://www.cdc.gov/nceh/demil/files/Federal%20Register%20Mustard%20AEL%205_2004.pdf; and int. MRL for H from 2003, in ATSDR 2005, http://www.atsdr.cdc.gov/mrls/index.html	Can persist in soil for months; subject to wet/dry deposition
Mustard sulfone	*471-03-4*	*(0.02)*	Protectively represented by the H/HD value above (CDC, ATSDR)	CDC 2004 (as above for H), http://www.cdc.gov/nceh/demil/files/Federal%20Register%20Mustard%20AEL%205_2004.pdf; and int. MRL for H from 2003, in ATSDR 2005, http://www.atsdr.cdc.gov/mrls/index.htm	Can persist in soil for months; subject to wet/dry deposition
Mustard, sulfur, distilled, with T (agent HT: mixture of 60% HD, 40% T)	Agent T = CAS 6392-89-8; Agent HD = CAS 505-60-2	0.02	GPL (CDC, ATSDR)	ATSDR 2005 and CDC 2004, as above for agents H and HD; T note CDC (2004) points out that "… toxicity data for agent T are inadequate for setting exposure limits … very low vapor pressure for agent T… precludes it as a vapor hazard under normal ambient conditions. For sulfur mustard and T mixtures, air monitoring for sulfur mustard alone should be sufficient under most circumstances to prevent airborne exposure to it."	More persistent than HD (>2 d); for the HD fraction, see HD/H above
Mustard sulfoxide	*5819-08-9*	*(0.02)*	Protectively represented by the H/HD value above (CDC, ATSDR)	CDC 2004 (as above for HD), http://www.cdc.gov/nceh/demil/files/Federal%20Register%20Mustard%20AEL%205_2004.pdf; and int. MRL from 2003, in ATSDR 2005, http://www.atsdr.cdc.gov/mrls/index.htm	Can persist in soil for months; subject to wet/dry deposition

Table 5 Risk-Based Criteria for the Initial Priority Chemicals and Their Key Transformation Products in Air

Chemical	CAS RN	Air Concn. *(µg/m³)*	Basis	Citation/Link for Risk-Based Value	Fate Notes
Mustard sulfone	*471-03-4*	*(0.02)*	Protectively represented by the H/HD value above (CDC, ATSDR)	CDC 2004 (as above for HD), http://www.cdc.gov/nceh/demil/files/Federal%20Register%20Mustard%20AEL%205_2004.pdf; and int. MRL from 2003, in ATSDR 2005, http://www.atsdr.cdc.gov/mrls/index.htm	Can persist in soil for months; subject to wet/dry deposition
Phorate	298-02-2	*No specific air benchmark found; this entry is included to introduce a fate product for which a benchmark exists (note that for inhalation exposures, the EPA 2006 OPP Interim reregistration eligibility decision (IRED) for Phorate considered a chronic oral NOAEL of 0.05 mg/kg-d, assumed full absorption; could suggest upper bound target of 1.75 µg/m³ with 100 for interspecies-intraspecies factors alone.) This estimate is consistent with the recommended chronic RfD of 0.0005 mg phorate/kg-d presented in Table 2, p. 10 of the OPP final Interim Reregistration Eligibility Decision (see www.epa.gov/oppsrrd1/reregistration/REDs/phorate_ired.pdf)*			Half-life for hydroxyl radical oxidation is <1.5 hr, 30 min for photolysis; in moist air, can hydrolyze with a 30- to 60-d half-life to the chemicals below
Hydrogen sulfide (H_2S)	*7783-06-4*	*2*	RfC, 2 µg/m³ (EPA IRIS)	EPA (2003), http://www.epa.gov/iris/subst/0061.htm; the CREL is 10 µg/m3, Cal/EPA 2005b *(listed in 2000)*, http://www.arb.ca.gov/toxics/healthval/contable.pdf; note the draft intermediate MRL is 28 µg/m3 (see www.atsdr.cdc.gov/mrls/index.html)	Hydrolysis product in moist air; oxidizes to hydrogen sulfate
Hydrogen sulfate (H_2SO_4), or sulfuric acid	*7664-93-9*	*1*	CREL (Cal/EPA)	Cal/EPA 2005b *(this CREL was listed in 2001)*, http://www.arb.ca.gov/toxics/healthval/contable.pdf	Oxidation product in moist air; dissociates to sulfate
Sulfate (SO^{2-}_4) (Cal/EPA CAS)	*9-96-0*	*25*	CREL (Cal/EPA)	Cal/EPA 2005b *(this CREL was listed in 1992)*, http://www.arb.ca.gov/toxics/healthval/contable.pdf	Terminal product can persist in air, is subject to deposition
Formaldehyde	*50-00-0*	*0.08*	IUR, 0.000013 per µg/m³ at 10^{-6} risk, for a risk-specific level of 0.08 µg/m³ (EPA IRIS)	EPA (1991a), http://www.epa.gov/iris/subst/0419.htm, for 10^{-6} risk level; chronic MRL of 0.008 ppm is 9.8 µg/m³ *(from 1999)*, and the CREL is 3 µg/m³ *(from 2005)*, in Cal/EPA 2005a, http://www.oehha.ca.gov/air/chronic_rels/pdf/50000.pdf	Hydrolysis product in moist air; photolysis half-life is 4–6 hr; can react with radicals to produce formic acid and carbon monoxide
Carbon monoxide (CO)	*630-08-0*	*10,000*	NAAQS for CO (EPA OAQPS)	EPA 1997b, http://www.epa.gov/air/criteria.html; note that this standard *(from 1990)* is an 8-hr average annual ceiling value	Can persist for several weeks; can oxidize to CO_2
Sarin (agent GB)	107-44-8	0.001	GPL (CDC)	CDC 2003 (Final Recommendations for Protecting Human Health from Potential Adverse Effects of Exposure to Agents GA (Tabun), GB (Sarin), and VX) http://a257.g.akamaitech.net/7/257/2422/14mar20010800/edocket.access.gpo.gov/2003/03-25583.htm	Photodegradation does not appear significant; hydroxyl radical half-life is 10 hr; half-life for hydrolysis in moist air is 3 d, forming HF and IMPA
Hydrogen fluoride (HF)	*7664-39-3*	*14*	CREL, (Cal/EPA)	Cal/EPA 2003 (*Adoption of Chronic Reference Exposure Levels for Fluorides including Hydrogen Fluoride*), http://www.oehha.ca.gov/air/chronic_rels/HyFluoCREL.html note that the value for F (vs. HF) is 13 µg/m³ (also note that the ATSDR acute MRL is 0.02 ppm or 16 µg/m³	Primary GB hydrolysis product in moist air, with IMPA, which only very slowly hydrolyzes to MPA and isopropanol; subject to wet/dry deposition

Table 5 Risk-Based Criteria for the Initial Priority Chemicals and Their Key Transformation Products in Air

Chemical	CAS RN	Air Concn *($\mu g/m^3$)*	Basis	Citation/Link for Risk-Based Value	Fate Notes
Methylphosphonic acid (MPA)	*993-13-5*	*24*	Estimated RfC (Munro/CHPPM); re-confirmed by Talmage et. al. (2007)	Munro et al. 1999, http://ehp.niehs.nih.gov/members/1999/107p933-974munro/munrotab16B.GIF; and Talmage et al (2007)	Forms very slowly from IMPA in moist air (estimated 1,900 yr half-life); is chemically stable
Isopropanol (isopropyl alcohol)	*67-63-0*	*7,000*	CREL (Cal/EPA)	Cal/EPA 2005b *(level established in 2000)*, http://www.arb.ca.gov/toxics/healthval/contable.pdf	Residence time in air is 1–2 d; hydroxyl radical oxidation forms acetone, acetaldehyde
Soman (agent GD)	96-64-0	0.001	GPL (Army Office of the Assistant Secretary)	DA (2004). "Interim Guidance Policy for New Airborne Exposures Limits for GB, GA, GD, GF, VX, H, HD and HT." Department of the Army, Office of the Assistant Secretary (Installations and Environment). 110 Army Pentagon, Washington, DC (18 Jun 2004).	Hydroxyl radical half-life is 8 hr; can hydrolyze in moist (alkaline) air, within min-hr to pinacolyl MPA and HF
Hydrogen fluoride (HF)	*7664-39-3*	*14*	CREL, 14 $\mu g/m^3$ (Cal/EPA)	Cal/EPA 2003 (as listed under sarin, above), http://www.oehha.ca.gov/air/chronic_rels/HyFluoCREL.html (for further context, see entry for HF under sarin above)	Primary hydrolysis product of GD, can form in moist air; subject to wet/dry deposition
Methylphosphonic acid (MPA)	*993-13-5*	*24*	Estimated RfC (Munro/CHPPM); reconfirmed by Talmage et al (2007)	Munro et al. 1999, http://ehp.niehs.nih.gov/members/1999/107p933-974munro/munrotab16B.GIF; and Talmage et al (2007)	Forms very slowly in moist air (estimated 1,900 yr half-life); is itself chemically stable
Tabun (agent GA)	*77-81-6*	*0.001*	GPL (CDC)	CDC 2003 (Final Recommendations for Protecting Human Health from Potential Adverse Effects of Exposure to Agents GA (Tabun), GB (Sarin), and VX) as for agent GB, sarin above), at http://a257.g.akamaitech.net/7/257/2422/14mar20010800/edocket.access.gpo.gov/2003/03-25583.htm	Hydroxyl radical half-life is 5 hr; can hydrolyze in moist air to compounds below, with a half-life of 8 hr at 20°C and pH 7.4, 14–28 hr at pH 7, 25°C
Dimethylamine	*124-40-3*	*2*	Early CREL (Cal/EPA); DMA not currently (2005) listed as CREL	Early CREL, Cal/EPA *(2000)*, http://www.oehha.ca.gov/risk/pdf/APENDX-B.pdf	Hydrolysis product in moist air, as is ethylphosphoryl cyanidate, which forms HCN; the hydroxyl radical half-life is 6 hr, faster in polluted air
Hydrogen cyanide (HCN)	*74-90-8*	*3*	RfC (EPA IRIS)	EPA (1994), http://www.epa.gov/iris/subst/0060.htm; based on cyanide toxicity (see Table 6 entry for further fate products)	From hydrolysis in moist air; subject to wet/dry deposition; hydroxyl radical half-life 1–3 yr
Cyanide (CN^-), free	*57-12-5*	*9*	CREL (Cal/EPA)	Cal/EPA 2005b for inorganic cyanide compounds (reviewed in 2000), http://www.arb.ca.gov/toxics/healthval/contable.pdf	Dissociation product, coexists with most as HCN in moist air
Phosphoric acid	*7664-38-2*	*10*	RfC, 0.01 mg/m^3 (EPA/IRIS)	RfC, 0.01 mg/m^3 from EPA/IRIS, EPA *(1995)*, http://www.epa.gov/irish/subst/0697.htm; CREL is 7 microgram/m^3 from Cal/EPA 2005b, http://www.arb.ca.gov/toxics/healthval/contable.pdf	Can form in moist air, can persist as terminal product

Table 5 Risk-Based Criteria for the Initial Priority Chemicals and Their Key Transformation Products in Air

Chemical	CAS RN	Air Concn. *(μg/m³)*	Basis	Citation/Link for Risk-Based Value	Fate Notes
Trimethyl phosphite (TMP)	*121-45-9*	*No specific air benchmark found; this entry is included to introduce the fate product for which a benchmark exists*			Can form methanol and DMP in moist air, hydrolysis limited by solubility, half-life is 4–10 d
Dimethyl phosphite (DMP or DMHP)	*868-85-9*	*420*	est. RfC, route-extrapolated from est. RfD (NAS-NRC)	NAS 2000a (provisional RfC from estimated RfD of 0.12 mg/kg-d), http://books.nap.edu/catalog.php?record_id= 9841, reflects conservative assumptions until more data are available	Can hydrolyze to phosphorous acid and methanol in moist air; hydrolysis half-life is 10–19 d
Methanol	*67-56-1*	*4,000*	CREL (Cal/EPA)	Cal/EPA 2005a *(current list; this CREL established in 2000)*, http://www.oehha.ca.gov/air/chronic_rels/pdf/67561.pdf	Hydrolysis product can form in moist air; hydroxyl radical half-life is 3–30 d
Phosphoric acid	*7664-38-2*	*10*	RfC, 0.01 mg/m³ (EPA/IRIS)	RfC, 0.01 mg/m³ from EPA/IRIS, EPA *(1995)*, http://www.epa.gov/irish/subst/0697.htm; CREL is 7 microgram/m³ from Cal/EPA 2005b, http://www.arb.ca.gov/toxics/healthval/contable.pdf	Can form in moist air; can persist as terminal fate product
VX, or: *O*-ethyl-*S*-[2-(diisopropylamino)ethyl] methylphosphonothioate	50782-69-9	0.0006	GPL (CDC)	CDC 2003 (Final Recommendations for Protecting Human Health from Potential Adverse Effects of Exposure to Agents GA (Tabun), GB (Sarin), and VX) as for agent GB, sarin above, at http://a257.g.akamaitech.net/7/257/2422/14mar20010800/edocket.access.gpo.gov/2003/03-25583.htm	Moderately persistent at 2 d to 1 wk; 57-hr half-life at neutral pH; in moist air can form EA 2192 and ethanol (ph >7) or DESH and EMPA (pH <6); 3-hr hydroxyl radical half-life
S-[2-(diisopropylamino)ethyl] methylphosphonothioic acid (EA 2192)	*73207-98-4*	*0.0007*	Estimated RfC (Munro, Talmage/CHPPM)	Munro et al. 1999 (solid compound and non-volatile), http://ehp.niehs.nih.gov/members/1999/107p933-974munro/munrotab16B.GIF; and Talmage et al (2007)	Primary hydrolysis product; from distilled water tests (per moist air), ~half follows this pathway; resists hydrolysis
Diisopropyl ethyl mercaptoamine (DESH)	*5842-07-9*	*4.6*	Estimated RfC (Munro, Talmage/CHPPM)	Munro et al. 1999, http://ehp.niehs.nih.gov/members/1999/107p933-974munro/munrotab16B.GIF; and Talmage et al. (2007)	Primary hydrolysis product; in distilled water tests, about a third follows this pathway; is more persistent than VX
O-ethyl methylphosphonic acid (EMPA)	*1832-53-7*	*34*	Estimated RfC (Talmage/CHPPM)	Munro et al. 1999, http://ehp.niehs.nih.gov/members/1999/107p933-974munro/munrotab16B.GIF; and Talmage et al. (2007)	Primary hydrolysis product; in distilled water tests, about a third follows this pathway; hydrolyzes very slowly to MPA and ethanol
Methylphosphonic acid (MPA)	*993-13-5*	*24*	Estimated RfC (Munro, Talmage/CHPPM)	Munro et al. 1999, http://ehp.niehs.nih.gov/members/1999/107p933-974munro/munrotab16B.GIF; and Talmage et al. (2007)	Hydrolysis product of EMPA, MPA itself is chemically stable
2-Diisopropylaminoethanol	*96-80-0*	*10*	Estimated RfC (Munro, Talmage/CHPPM)	Munro et al. 1999, http://ehp.niehs.nih.gov/members/1999/107p933-974munro/munrotab16B.GIF; and Talmage et al. (2007)	Primary hydrolysis product of VX, persistence expected to be similar to DESH
O-ethylmethylphosphonothioic acid (EMPTA)	*18005-40-8*	*8.5*	Estimated RfC (Munro, Talmage/CHPPM)	Munro et al. 1999, http://ehp.niehs.nih.gov/members/1999/107p933-974munro/munrotab16B.GIF; and Talmage et al. (2007)	Primary hydrolysis product of VX, can oxidize to EMPA

[a] Table 5 identifies risk-based criteria that address priority chemicals and key transformation products for which benchmarks were found; 3 of these threat chemicals are represented by their fate products – ethyldichloroarsine (ED), phorate, and trimethyl phosphite (TMP) – and no relevant benchmarks were found for tetraethyl pyrophosphate, (TEPP). Fate products are indented in italics, and only those with relevant benchmarks are shown. Some products common to more than one primary contaminant, while others are unique. For VX, associated impurities not in the NHSRC list or SAM report are not included; for those other chemicals, see Munro et al. (1999) and Talmage et al. (2007).

Except as indicated, these concentrations represent long-term (repeated or continuous) exposures. Parentheses identify derived concentrations, e.g., from values for related chemicals. Calculated values are rounded to two significant figures. MOE = margin of exposure. Under standard conditions, $mg/m^3 = (molecular\ weight/24.5) \times ppm$.

EPA benchmarks are prioritized, with others included as further context; lower values shown in lighter font (green). The IRIS database was initially accessed in 2005 and checked again in September 2007 as this document was completed. Italicized dates shown in parentheses here and in subsequent tables represent when the benchmarks were established (or in some cases further reviewed), so that time frame can be appreciated when comparing with other benchmarks established earlier or later. For example, while the current set of CRELs is dated 2005, the years in which individual limits were formalized are also shown in these tables. Similarly, from the December 2006 MRL list, the dates individual limits were established rather than that most recent overall publication date are presented in these tables.

No direct chronic public benchmarks were found for the following chemicals in this review: dicrotophos, ED, fenamiphos, mevinphos, nicotine, phorate, strychnine, TEPP, and TMP. Parentheses are used to distinguish preliminary indicators derived for dicrotophos and fenamiphos from information developed for long-term inhalation by the EPA Office of Prevention, Pesticides, and Toxic Substanes (OPPTS), notably the Office of Pesticide Programs (OPP), which suggests method validation targets could be further below those levels. Similarly, italicized values in parentheses for several fate products represent generally conservative preliminary indicators, as they reflect benchmarks for parent compounds that are considered more toxic.

To further address gaps, acute exposure levels and data for similar chemicals were also checked for insights into possible bounding context and relative toxicity. As a note for ED, a 1 hr AEGL 2 of 29 $\mu g/m^3$ is an interim inhalation value above (see EPA website http://www.epa.gov/oppt/aegl/pubs/rest136.html); thus it would be considered a very high bound, e.g., method validation to support final decontamination levels for chronic exposures would be expected to target a much lower concentration.

Chemical Abstracts Service Registry Number [American Chemical Society] (CAS/RN)

Table 6 Risk-Based Criteria for Additional Chemical Agents and Their Key Transformation Products in Air

Chemical	CAS RN	Air Concn. *(μg/m^3)*	Basis	Citation/Link for Risk-Based Value	Fate Notes
Arsine (agent SA)	7784-42-1	0.05	RfC (EPA IRIS)	EPA *(1994)*, http://www.epa.gov/iris/subst/0672.htm; this is also the CREL *(from 1996)* in Cal/EPA 2005b, http://www.arb.ca.gov/toxics/healthval/contable.pdf	Does not persist beyond min-hr; decomposes in moist air and light to deposit elemental arsenic; can explode on contact with warm, dry air; can hydrolyze to arsenic acids, hydrides; can oxidize to trivalent, pentavalent arsenic compounds that settle out (deposit on surfaces)
Arsenic, inorganic	*7440-38-2*	*0.0002*	Estimated air concentration resulting in 1 x 10^{-6} risk; IUR at 0.0043 per μg/m^3, (EPA IRIS)	No RfC for inorganic arsenic established by EPA; EPA *(1998)*, http://www.epa.gov/iris/subst/0278.htm CREL is 0.03 μg/m^3 *(listed in 2001)*, evaluated in Cal/EPA *(2005b)*, http://www.oehha.ca.gov/air/chronic_rels/pdf/arsenics.pdf	Oxidation product; atmospheric lifetime could be 5 to 15 d with loss due to deposition
Cyanogen chloride (agent CK)	506-77-4	9.0	CREL for inorganic cyanide compounds, 9.0 μg/m^3 (Cal/EPA)	The CREL for inorganic cyanide compounds is 9.0 μg/m^3 *(listed in 2000)*, in Cal/EPA 2005b, http://www.oehha.ca.gov/air/chronic_rels/pdf/7782505.pdf	Persists only 1–10 min in air; reacts with hydroxyl radicals to liberate hydrogen; can hydrolyze in moist air to form cyanic acid, HCl (half-life is 1 min at 45°C, 10 hr at 5°C)
Hydrogen chloride (HCl)	7647-01-0	*20*	RfC, 0.02mg/m^3 (EPA IRIS)	EPA *(1995a)*, http://www.epa.gov/iris/subst/0396.htm; non-EPA value is lower, CREL 9 μg/m^3 *(2000)* in Cal/EPA 2005b, http://www.oehha.ca.gov/air/chronic_rels/pdf/7647010.pdf	Hydrolysis product, would be incorporated into moisture in air; subject to wet/dry deposition
Ammonia (NH_3)	*7664-41-7*	*100*	RfC, 0.1 mg/m^3 (EPA IRIS)	EPA *(1991a)*, http://www.epa.gov/iris/subst/0422.htm; a non-EPA value is lower, the MRL of 0.1 ppm or 70 μg/m^3, ATSDR 2005, http://www.atsdr.cdc.gov/mrls.html; ammonia CREL 200 μg/m^3, anhydrous-aqueous *(listed 2000)*, Cal/EPA 2005b, http://www.oehha.ca.gov/air/chronic_rels/pdf/7664417.pdf	Formed from the cyanic acid (HOCN) hydrolysis product, along with CO_2; the vapor can persist for about 1 wk
Cyclohexyl sarin (agent GF, or cyclosarin)	329-99-7	0.001	GPL (Army Office of the Assistant Secretary)	DA (2004). "Implementation Guidance Policy for New Airborne Exposures Limits for GB, GA, GD, GF, VX, H, HD and HT." Department of the Army, Office of the Assistant Secretary (Installations and Environment). 110 Army Pentagon, Washington, D.C. (18 Jun 2004)	Hydroxyl radical reaction half-life is 2 d; this is also the hydrolysis half-life in moist air at 25°C
Hydrogen fluoride (HF)	*7664-39-3*	*14*	CREL (Cal/EPA)	Cal/EPA 2003 (*Adoption of Chronic Reference Exposure Levels for Fluorides Including Hydrogen Fluoride*), http://www.oehha.ca.gov/air/chronic_rels/HyFluoCREL.html note that the value for F (versus HF) is 13 μg/m^3 (also note that the ATSDR acute MRL is 0.02 ppm or 16 μg/m^3)	Primary hydrolysis product of GF, can form in moist air along with cyclohexyl MPA; subject to wet/dry deposition

Table 6 Risk-Based Criteria for Additional Chemical Agents and Their Key Transformation Products in Air

Chemical	CAS RN	Air Concn *(µg/m³)*	Basis	Citation/Link for Risk-Based Value	Fate Notes
Methylphosphonic acid (MPA)	*993-13-5*	*24*	Estimated RfC (Munro/CHPPM); re-confirmed by Talmage et al *(2007)*	Munro et al. 1999, http://ehp.niehs.nih.gov/members/1999/107p933-974munro/munrotab16B.GIF; and Talmage et al *(2007)*	Hydrolysis product, forms very slowly from cyclohexyl methyl-phosphonic acid; MPA is stable
Ethyl sarin (agent GE)	1189-87-3	NA	No specific values found for GE.	No specific values found for GE. In the absence of any available literature from which to draw a relative potency comparison with any other nerve agent, it is recommended that no risk-based criteria be provided at this time. If data or analyses can be made available, this compound can be re-visited.	Not available. In the absence of compound-specific fate data for agent GE or documented comparison with agent GB degradation, it is recommended that no fate reactions be presented at this time. When data or analyses become available, this compound can be re-visited.
Hydrogen cyanide (HCN, agent AC)	74-90-8	3	RfC (EPA IRIS)	EPA 1994, http://www.epa.gov/iris/subst/0060.htm; based on cyanide toxicity	Can disperse rapidly; resists degradation, with atmospheric residence time of 1–3 yr depending on hydroxyl radical concentration
Cyanide (CN), free	*57-12-5*	*9*	CREL (Cal/EPA)	Cal/EPA 2005b, for inorganic cyanide compounds (reviewed in 2000) http://www.arb.ca.gov/toxics/healthval/contable.pdf	Dissociation product, coexists with most as HCN in moist air
Nitrogen dioxide (NO_2)	*10102-44-0*	*100*	NAAQS for NO_2 (EPA OAQPS)	EPA 1997b, http://www.epa.gov/air/criteria.html; note that the air quality standard *(from 1990)* is the annual arithmetic mean; CREL is 470 µg/m³ *(from 1992)*, in Cal/EPA 2005b, http://www.arb.ca.gov/toxics/healthval/contable.pdf	Hydroxyl radical oxidation of HCN forms nitric oxide (NO), which rapidly interconverts with NO_2 in sunlight; can form nitrous and nitric acids in moist air
Nitric acid (HNO_3)	*7697-37-2*	*(86); (acute only)*	AREL (Cal/EPA)	Cal/EPA *(2000)*, only for *acute*, no chronic level found, http://www.oehha.org/air/acute_rels/allAcRELs.html	Product of NO_2 reaction in moist air; subject to wet/dry deposition
Carbon monoxide (CO)	*630-08-0*	*10,000*	NAAQS for CO (EPA OAQPS)	EPA 1997b, http://www.epa.gov/air/criteria.html; note that this standard *(from 1990)* is an 8-hr average annual ceiling value	Can oxidize to CO_2; can persist for several weeks
Mustard, nitrogen (HN-2)	51-75-2	*No specific air benchmark found; this entry is included to introduce the fate product for which a benchmark exists*			Hydroxyl radical reaction half-life 5 hr to 2 d; dimerizes; hydrolyzes to HCl and N methyldiethanolamine with a half-life of 11 hr
Hydrogen chloride (HCl)	*7647-01-0*	*20*	RfC, 0.02 mg/m³ (EPA IRIS)	EPA *(1995a)*, http://www.epa.gov/iris/subst/0396.htm; non-EPA value is lower, CREL 9 µg/m³ (2000) in Cal/EPA 2005a, http://www.oehha.ca.gov/air/chronic_rels/pdf/7647010.pdf	Hydrolysis product, is incorporated into moisture in air; subject to wet/dry deposition

Table 6 Risk-Based Criteria for Additional Chemical Agents and Their Key Transformation Products in Air

Chemical	CAS RN	Air Concn. *(µg/m^3)*	Basis	Citation/Link for Risk-Based Value	Fate Notes
Perfluoroisobutylene (PFIB)	382-21-8	(0.3)	Estimated as approximately equivalent to phosgene RfC of 0.3 µg/m^3 (EPA IRIS)	EPA *(2006f)*, http://www.epa.gov/iris/subst/0487.htm; estimated as approximately equivalent to phosgene RfC based on comparison of Provisional Advisory Level (PAL) concentrations for PFIB and phosgene under current review by NHSRC	Thermal by-product of Teflon synthesis (same precursors); in moist air, can hydrolyze to fluorophosgene, forms CO_2 and HF
Hydrogen fluoride (HF)	*7664-39-3*	*14*	CREL (Cal/EPA)	Cal/EPA 2003 *(Adoption of Chronic Reference Exposure Levels for Fluorides Including Hydrogen Fluoride)*, http://www.oehha.ca.gov/air/chronic_rels/HyFluoCREL.html (for further context, see entry for HF under agent GE above)	Secondary hydrolysis product, can form in moist air; subject to wet/dry deposition
Red phosphorus (RP)	7723-14-0	(10)	Related RfC for phosphoric acid, 10 µg/m^3 (from RP combustion products) (EPA IRIS); NRC *(1997)*	EPA *(1995a)*, http://www.epa.gov/iris/subst/0697.htm; note that this RfC for phosphoric acid is based on RP combustion products (likely exposure condition and consistent with NRC *[1997]* appraisal that phosphoric acid is key toxic component of RP fume), which include phosphorous and phosphoric acids. The CREL for phosphoric acid is 7 microgram/m^3 (Cal/EPA 2005b)(listed in 2000). For comparison, the CREL for phosphoric acid is 7.0 micrograms/m^3 and that for the more toxic white P (WP) is 0.07 µg/m^3, Cal/EPA 2005b *(listed in 1991)*, http://www.arb.ca.gov/toxics/healthval/contable.pdf	Highly flammable solid, reacts slowly with water vapor and oxygen to produce phosphine in air (estimated half-life >3,500 yr), accelerated by metals and oxidizers
Phosphine	*7803-51-2*	*0.3*	RfC, 0.0003 mg/m^3 (EPA IRIS)	EPA *(1995a)*, http://www.epa.gov/iris/subst/0090.htm; the CREL is 0.8 µg/m^3 *(listed in 2002)*, in Cal/EPA 2005a, http://www.oehha.ca.gov/air/chronic_rels/pdf/7803512.pdf	Hydrolysis product, can form in moist air; hydroxyl radical half-life is about 1 d
Phosphoric acid	*7664-38-2*	*10*	RfC, 0.01 mg/m^3 (EPA IRIS)	RfC of 0.01 mg/m^3 from EPA/IRIS, EPA *(1995)*, http://www.epa.gov/iris/subst/0697.htm; CREL is 7 microgram/m^3 from Cal/EPA 2005b, http://www.arb.ca.gov/toxics/healthval/contable.pdf	Can form in moist air; can persist as a terminal fate product
Tear gas (agent CS)	2698-41-1	(0.03)	Protectively represented by the RfC, 0.00003 mg/m^3 for the tear gas form CN (EPA IRIS)	EPA *(1991a)* (this RfC is for the tear gas form CN, or 2-chloroacetophenone, CAS number 532-27-4), http://www.epa.gov/iris/subst/0537.htm; tear gas form CS is less toxic than tear gas form CN, per Rega et al. 2006, http://www.emedicine.com/emerg/topic914.htm, and others	Can hydrolyze in moist air in minutes, to 2-chlorobenzaldehyde and malononitrile (relatively toxic); note: in the body (but not in air), converts to cyanide and thiocyanate
Titanium tetrachloride (FM)	7550-45-0	0.1	Chronic MRL, 0.0001 mg/m^3 (ATSDR)	ATSDR 1997d, http://www.atsdr.cdc.gov/toxprofiles/tp101.html	Disperses readily; in moist air can hydrolyze to produce smoke of HCl and titanium oxychloride and hydroxide, with half-life of hours

Table 6 Risk-Based Criteria for Additional Chemical Agents and Their Key Transformation Products in Air

Chemical	CAS RN	Air Concn. *(μg/m³)*	Basis	Citation/Link for Risk-Based Value	Fate Notes
Hydrogen chloride (HCl)	*7647-01-0*	*20*	RfC, 0.02 mg/m³ (EPA IRIS)	EPA *(1995a)*, http://www.epa.gov/iris/subst/0396.htm; non-EPA value lower, CREL 9 μg/m³ *(2000)* in Cal/EPA 2005a, http://www.oehha.ca.gov/air/chronic_rels/pdf/7647010.pdf	Hydrolysis product, is incorporated into moisture in air; subject to wet/dry deposition
VG, Amiton, or: O,O-diethyl-S [2 (diethylamino) ethyl] phosphorothioate	78-53-5	*No specific air benchmark was found; this entry is included to introduce a fate product for which a specific benchmark exists*			Hydrolysis fate of Amiton (agent VG) is not well-characterized and it is unclear if data for nerve agent VX represent a reasonable surrogate.
Phosphoric acid	*7664-38-2*	*10*	RfC, 0.01 mg/m³ (EPA IRIS)	RfC of 0.01 mg/m³ from EPA/IRIS, EPA *(1995)*, http://www.epa.gov/iris/subst/0697.htm; CREL is 7 microgram/m³ from Cal/EPA 2005b, http://www.arb.ca.gov/toxics/healthval/contable.pdf	Potential fate product; can form in moist air; can persist as a terminal fate product
VM, or: *O*-ethyl-*S*-[2-(diethylamino)ethyl] methylphosphonothioate	21770-86-5	*No compound-specific information is available, so an assumption cannot be made about toxicity.*			In the absence of specific degradation information for VMs are not assessed.
Vx, or: *O*-ethyl-*S*-[2-(dimethylamino)ethyl] methylphosphonothioate	20820-80-8	*No specific benchamark found.*		"No toxicity estimates are recommended at this time because data are lacking"; Dept. of the Army (2005), Potential Military Chemical/Biological Agents and Compounds. FM 3-11.9, US Dept. of the Army, Pentagon, Washington, DC (approved for public release, distribution unlimited)	In the absence of specific degradation information for Vsubx, fate products are not assessed.

[a] This table identifies concentrations addressing additional chemical agents and key transformation products (indented, in italics); 2 are represented by potential fate products: nitrogen mustard, and VG; no relevant benchmarks were identified for VE. Some fate products are common to more than one primary contaminant while others are unique. Unless otherwise noted, concentrations represent limits for long-term exposures. EPA benchmarks are prioritized, with others included as further context; lower values are shown in lighter font (green). Parentheses identify derived concentrations, from related chemicals. Calculated values are rounded to two significant figures. To convert concentrations under standard conditions: *mg/m³ = (molecular weight/24.5)* × *ppm*. For those without relevant public benchmarks, occupational limits were also assessed to provide initial context. For example, although no public guideline was found specifically for HN-2, the CDC identifies a workplace airborne exposure limit (AEL) of 3 μg/m³ for nitrogen mustard HN-1, and the acute toxicity of HN-2 is half that of HN-1 (*from the Medical Management Guidelines for Blister Agents, Nitrogen Mustards,* ATSDR 2006). Note that the AEL is "a maximum concentration of an agent in air that is safe for continuous exposure during an 8-hr work day" and is considered a general term indicating a level of exposure unlikely to result in adverse health effects (NAS 2000b).

Table 7 Risk-Based Criteria for the Initial Priority Chemicals and Their Key Transformation Products in Water

Chemical	CAS RN	Water Concn. *(µg/L)*	Basis	Citation/Link for Risk-Based Value	Fate Notes
Chloropicrin	76-06-2	50	Archived Action Level, 0.05mg/L CA Dept of Health Services	CA Department of Health Services (2007), http://www.dhs.ca.gov/ps/ddwem/chemicals/AL/PDFs/archive.pdf, archived advisory level	Little to slow hydrolysis, with a half-life of 11 yr; photolysis half-life is 3 d (surface water), with volatilization half-life 4 hr to 5 d
Nitrate (NO$_3$), as N	*14797-55-8*	*10,000*	MCL, 10mg/L (EPA Office of Water)	EPA 2004a, 1992 MCL, 10 mg/L, http://www.epa.gov/safewater/contaminants/index.html. EPA *(1991a)*, http://www.epa.gov/iris/subst/0076.htm, RfD is for an infant at 0.64 L/d (70-kg adult, 2 L/d, would be 56,000 µg/L); this value is equal to the 1992 MCL	Photolysis product (e.g., in open systems); nitrogen naturally cycles in the environment
Nitrite (NO$_2$), as N	14797-65-0	1,000	MCL, 1 mg/L (EPA Office of Water)	EPA 2004a, 1992 MCL, 1 mg/L, http://www.epa.gov/safewater/contaminants/index.html. EPA *(1997)*, http://www.epa.gov/iris/subst/0078.htm, for the 10-kg child (70-kg adult, 2 L/d, would be 3,500 µg/L); this value is equal to the 1992 MCL	Photolysis product (e.g., in open systems), from nitrate; nitrogen naturally cycles in the environment
Dichlorvos	62-73-7	0.28	SF, 0.29 per mg/kg-d (EPA IRIS)	EPA *(1993)*, http://www.epa.gov/iris/subst/0151.htm; RfD is 0.0005 mg/kg-d (18 µg/L), same as MRL; EPA (2006d), Interim Reregistration Eligibility Decision for Dichlorvos (DDVP), http://www.epa.gov/pesticides/reregistration/REDs/ddvp_ired.pdf, is OPP RfD, with chronic NOAEL of 0.05 mg/kg-d and UF of 100	Hydrolysis half-life is 4 d at pH 7 (decreases with increasing pH); volatilization half-life is on the order of months
Dichloroacetic acid	*79-43-6*	*60*	Represented by toxicity of Haloacetic acids, MCL, 0.06 mg/L (EPA Office of Water)	EPA 2004a, MCL, 0.06 mg/L, http://www.epa.gov/safewater/contaminants/index.html. On this MCL website, EPA has a footnote for Haloacetic acids that states the MCL is used for all the compounds in this group. EPA *(2003)*, http://www.epa.gov/iris/subst/0654.htm; 95% upper bound for 10^{-6} risk, central tendency 2.3 µg/L; RfD 0.004 mg/kg-d is 140 µg/L; the DWEL is 100 µg/L	Hydrolysis product; the environmental half-life of this haloacetic acid (HAA) is <100 hr
Methanol	*67-56-1*	*18,000*	RfD, 0.5 mg/kg-d (EPA IRIS)	EPA *(1993)*, http://www.epa.gov/iris/subst/0305.htm	Hydrolysis product; volatilization half-life of 5–52 d
Phosphoric acid, phosphate	*7664-38-2*	*12,000*	Drinking water guideline, 12 ppm (Maui Department of Water Supply [DOWS])	Maui DOWS 2004 (based on 12 ppm 85% phosphoric acid solution as health protective, from American National Standards Institute [ANSI] and National Sanitation Foundation), http://mauiwater.org/phosphates.html	Terminal hydrolysis product; phosphates can persist
Dicrotophos (Bidrin)	141-66-2	3.5	RfD, 0.0001 mg/kg-d (EPA IRIS)	EPA *(1989)*, http://www.epa.gov/iris/subst/0211.htm; in EPA 2002a (OPPTS drinking water level of comparison), http://www.epa.gov/oppsrrd1/REDs/dicrotophos_ired.pdf, chronic general population DWLOC is 1 ppb, or 1 µg/L; the chronic drinking water level of comparison (DWLOC) for ages 1–6 is 0.2 ppb, or 0.2 µg/L	Hydrolysis half-life is 72 d at 25°C and pH 7, faster in alkaline water

Table 7 **Risk-Based Criteria for the Initial Priority Chemicals and Their Key Transformation Products in Water**

Chemical	CAS RN	Water Concn. *(µg/L)*	Basis	Citation/Link for Risk-Based Value	Fate Notes
Acetone	*67-64-1*	*32,000*	RfD, 0.9 mg/kg-d (EPA IRIS)	EPA *(2003)*, http://www.epa.gov/iris/subst/0128.htm	Hydrolysis product; volatilization half-life ranges from 8 hr to 14 d, readily biodegradable (1 d for aerobic, 5 d for anaerobic), adsorption not significant
Methanol	*67-56-1*	*18,000*	RfD, 0.5 mg/kg-d (EPA IRIS)	EPA *(1993)*, http://www.epa.gov/iris/subst/0305.htm	Hydrolysis product; volatilization half-life is 5-52 d
Phosphoric acid, phosphate	*7664-38-2*	*12,000*	Drinking water guideline, 12 ppm (Maui DOWS)	Maui DOWS 2004 (based on 12 ppm 85% phosphoric acid solution as health protective, from American National Standards Institute [ANSI] and National Sanitation Foundation), http://mauiwater.org/phosphates.html	Terminal hydrolysis product; phosphates can persist
Dimethyl phosphite (DMP)	*868-85-9*	*1,500*	SF, 0.0054 per mg/kg-d (NAS)	NAS 2000a (Organic Phosphonates, in Toxicological Risks of Selected Flame-Retardant Chemicals), http://www.nap.edu/books/0309070473/html/328.html; for a risk level of 10^{-4}, this translates to 1,500 µg/L; note that an RfD was also identified, as 0.12 mg/kg-d, which translates to 4,200 µg/L	Hydrolysis half-life 10 d at 25°C, slower in cooler water and higher pH; forms methanol and MP, which hydrolyzes to methanol and phosphorous acid, which oxidizes to phosphoric acid
Methanol	67-56-1	18,000	RfD, 0.5 mg/kg-d (EPA IRIS)	EPA *(1993)*, http://www.epa.gov/iris/subst/0305.htm	Hydrolysis product; volatilization half-life is 5–52 d
Phosphoric acid, phosphate	*7664-38-2*	*12,000*	Drinking water guideline, 12 ppm (Maui DOWS)	Maui DOWS 2004 (based on 12 ppm 85% phosphoric acid solution as health protective, from American National Standards Institute [ANSI] and National Sanitation Foundation), http://mauiwater.org/phosphates.html	Terminal oxidation product following MP hydrolysis to phosphorous acid; phosphates can persist
Ethyldichloroarsine (agent ED)	598-14-1	*No specific drinking water benchmark found; this entry is included to introduce the fate product for which a benchmark exists*			Poorly soluble in water, persists 1–6 d at 5–30°C; can react to form persistent solids
Arsenic (inorganic)	*7440-38-2*	*10*	MCL, 0.01 mg/L (EPA Office of Water)	EPA (2004a),The MCL is 10 ug/L (from 50 in 2001), http://www.epa.gov/safewater/contaminants/index.html, as is the DWEL; the IRIS drinking water unit risk (DWUR) is 0.00005 per ug/L, 0.02ug/L for 10-6 risk level, EPA *(1998)*, http://www.epa.gov/iris/subst/0278.htm; 1993 RfD of 0.0003 mg/kg-d *(also 2000 Cal/EPA, 1995 draft HA, 2005 MRL)* gives 11 µg/L (rounded)	Arsenoxides/inorganic arsenic can persist for years and can settle out within months (surface waters)
Fenamiphos	22224-92-6	8.8	RfD, 0.00025 mg/kg-d (EPA IRIS)	EPA *(1990)*, http://www.epa.gov/iris/subst/0240.htm; the earlier 1988 HA is 2 µg/L, DWEL is 9 µg/L (EPA 2004a); OPPTS RfD of 0.0001 mg/kg-d gives 3.5 µg/L, in EPA 1999a, OPPTS chronic DWLOC for general public is 4 ppb; 1 ppb (µg/L) for child (most sensitive group), EPA 2002b, http://www.epa.gov/pesticides/reregistration/REDs/fenamiphos_ired.pdf	Half-life in surface water from oxidation and photolysis is 1.8 d, much shorter with irradiation (<30 min); hydrolysis is slow, with a half-life of 200–300 d at pH 7

Table 7 **Risk-Based Criteria for the Initial Priority Chemicals and Their Key Transformation Products in Water**

Chemical	CAS RN	Water Concn *(µg/L)*	Basis	Citation/Link for Risk-Based Value	Fate Notes
Fenamiphos sulfoxide	*31972-43-7*	*(8.8)*	Represented by IRIS RfD of the parent, see previous entry (EPA IRIS)	EPA *(1990)*, http://www.epa.gov/iris/subst/0240.htm, and 2002b (conservatively represented by above); based on same excretion pattern, metabolites, from IPCS 1997, http://www.inchem.org/documents/jmpr/jmpmono/v097pr06.htm; also note OPPTS child DWLOC of 1 µg/L above	Oxidation products; the sulfoxide further oxidizes to the sulfone, and persistence can be similar to the parent
Fenamiphos sulfone	*31972-44-8*	*(8.8)*			
Phosphoric acid, phosphate	*7664-38-2*	*12,000*	Drinking water guideline, 12 ppm (Maui DOWS)	Maui DOWS 2004 (based on 12 ppm 85% phosphoric acid solution as health protective, from American National Standards Institute [ANSI] and National Sanitation Foundation), http://mauiwater.org/phosphates.html	Terminal hydrolysis product; phosphates can persist
Lewisite (Lewisite-1, agent L-1)	541-25-3	3.5	Estimated RfD, 0.0001 mg/kg-d (Army, NAS and Opresko et al.)	Opresko et al. 2001. Chemical Warfare Agents: Current Status of Oral Reference Doses. Rev Environ Contam Toxicol 172:65–85. According to this source, the estimated RfD for Lewisite is "appropriate when presence of L, CVAA, or Lewisite Oxide is known". (note NAS considered a value 10 times lower)	Slightly soluble; hydrolyzes quickly with a half-life of <2 min to 2-chlorovinylarsonous acid and HCl; the volatilization half-life is 8 hr to 1 wk
2-Chlorovinylarsonous acid (CVAA)	*85090-33-1*	*(3.5)*	Represented by toxicity of the parent, as above (Army, NAS and Opresko et al.)	Opresko et al. 2001 (as above), based on no appreciable difference in toxicity between L-1 and metabolite/LO equilibrium mixture, Noblis 2005, http://www.noblis.org/ChemistryOfLLewisite.htm	Primary hydrolysis product of L-1; undergoes dehydration to form lewisite oxide (LO) and LO polymers; slightly more environmentally stable than the parent lewisite, http://www.noblis.org/ChemistryOfLLewisite.htm
Lewisite oxide	*3088-37-7*	*(3.5)*	Represented by toxicity of parent, as above (Army, NAS and Opresko et al.)	Opresko et al. 2001, and per no appreciable toxicity difference, Noblis *(2005)*, http://www.noblis.org/ChemistryOfLLewisite.htm	Hydrolysis product of 2-chlorovinylarsonous acid, can dehydrate to lewisite oxide polymer; persists
Arsenic (inorganic)	*7440-38-2*	*10*	MCL, 0.01 mg/L (EPA Office of Water)	EPA (2004a), New MCL is 10 ug/L (from 50 in 2001), http://www.epa.gov/safewater/contaminants/index.html, as is the DWEL; the IRIS DWUR is 0.00005 per µg/L, 0.02 µg/L for 10^{-6} risk level, EPA *(1998)*, http://www.epa.gov/iris/subst/0278.htm; 1993 RfD of 0.0003 mg/kg-d *(also 2000 Cal/EPA, 1995 draft HA, 2005 MRL)* gives 11 µg/L *(rounded)*	Organic and inorganic products convert to arsenite and arsenate, can persist for years and settle out in months (surface waters)
Lewisite (Lewisite-2, agent L-2)	40334-69-8	(3.5)	Protectively bounded by the estimated RfD for L-1 (above) (Army, NAS and Opresko et al.)	Opresko et al. 2001 (see L-1 above; L-2 and L-3 are less toxic); estimated RfD	Hydrolyzes more slowly than L-1 to form HCl and bis(2-chlorovinyl)arsonous acid
Arsenic (inorganic)	*7440-38-2*	*10*	MCL, 0.01 mg/L (EPA Office of Water)	EPA (2004a) New MCL is 10 ug/L (from 50 in 2001), http://www.epa.gov/safewater/contaminants/index.html, as is the DWEL; IRIS DWUR is 0.00005 per ug/L. 0.02 ug/L for 10^{-6} risk level, EPA *(1998)*, http://www.epa.gov/iris/subst/0278.htm; 1993 RfD of 0.0003 mg/kg-d *(also 2000 Cal/EPA, 1995 draft HA, 2005 MRL)* gives 11 µg/L (rounded)	Organic and inorganic products convert to arsenite and arsenate, can persist for years and settle out in months (surface waters)

Table 7 Risk-Based Criteria for the Initial Priority Chemicals and Their Key Transformation Products in Water

Chemical	CAS RN	Water Concn. *(µg/L)*	Basis	Citation/Link for Risk-Based Value	Fate Notes
Lewisite (Lewisite-3, agent L-3)	40334-70-1	(3.5)	Protectively bounded by the estimated RfD for L-1 (above) (Army, Opresko et al.)	Opresko et al. 2001 (see L-1 above; L-2 and L-3 are less toxic); estimated RfD	Among agents, rated as persistent at 1–3 d; resists hydrolysis but volatilizes
Methyl parathion	298-00-0	8.8	RfD, 0.00025 mg/kg-d (EPA IRIS)	EPA *(1991a)*, http://www.epa.gov/iris/subst/0174.htm; EPA 2004a (same RfD, DWEL 9 µg/L, and 1988 HA 2 µg/L), http://www.epa.gov/waterscience/criteria/drinking/standards/dwstandards.pdf; MRL of 0.0003 mg/kg-d is 11 µg/L (10.5) (from 2001); note EPA (OPPTS) 2003b, http://www.epa.gov/oppsrrd1/REDs/methylparathion_ired.pdf, chronic RfD of 0.0002 mg/kg-d, gives 7 µg/L; with safety factor 10, OPPTS chronic population-adjusted dose is 0.7 µg/L and chronic child DWLOC is 0.18 µg/L *(1999)*	Hydrolysis half-life can be <1 to 4 wk or more, depending on temperature, pH, and other system conditions; forms para-nitrophenol (4-nitrophenol) and dimethylphosphorothioic acid
p-Nitrophenol (or para-nitrophenol)	*100-02-7*	*280*	RfD, 0.008 mg/kg-d (EPA Region 6) HA, lifetime, 0.06 mg/L (EPA Office of Water)	EPA Region 6 (2007) http://www.epa.gov/earth1r6/6pd/rcra_c/pd-n/screenvalues.pdf; also a HA, established in 1992, of 0.06 mg/L, http://www.epa.gov/waterscience/criteria/drinking/standards/dwstandards.pdf, report also lists RfD 0.008 mg/kg-d, for 280 µg/L (no RfD is in IRIS), and DWEL of 300 µg/L	Primary hydrolysis product, reduces to p-aminophenol; photolysis half-life in surface water is 6.7 d at pH 7
Methyl paraoxon	950-35-6	(0.88)	RfD for parathion above, toxicity-scaled (÷ 10) (EPA IRIS)	EPA 2004a (as above) and Cal/EPA 1999 *(Scientific Review Panel, Methyl Parathion)*, http://www.arb.ca.gov/srp/srp3.pdf; judged 10x more toxic than parent (inhalation, but per oral) scaled from IRIS RfD	Oxidation product; hydrolyzes within days at pH 8.5, much faster than the parent methyl parathion
Methanol	67-56-1	18,000	RfD, 0.5 mg/kg-d (EPA IRIS)	EPA *(1993)*, http://www.epa.gov/iris/subst/0305.htm	Hydrolysis product; volatilization half-life is 5–52 d
Phosphoric acid, phosphate	*7664-38-2*	*12,000*	Drinking water guideline, 12 ppm (Maui DOWS)	Maui DOWS 2004 (based on 12 ppm 85% phosphoric acid solution as health protective, from American National Standards Institute [ANSI] and National Sanitation Foundation), http://mauiwater.org/phosphates.html	Terminal hydrolysis product; phosphates can persist
Mevinphos	7786-34-7	8.8	RfD, 0.00025 mg/kg-d (EPA OPPTS)	EPA 2000b (chronic RfD, per NOAEL 0.025 mg/kg-d), http://www.epa.gov/oppsrrd1/REDs/0250tred.pdf	Hydrolysis half-life is 35 d at pH 7, 120 d at pH 6; hydrolyzes to methyl acetoacetate, dimethyl phosphate, and the two compounds below
Methanol	*67-56-1*	*18,000*	RfD, 0.5 mg/kg-d (EPA IRIS)	EPA *(1993)*, http://www.epa.gov/iris/subst/0305.htm	Hydrolysis product; volatilization half-life is 5–52 d
Phosphoric acid, phosphate	*7664-38-2*	*12,000*	Drinking water guideline, 12 ppm (Maui DOWS)	Maui DOWS 2004 (health-based level for 85% phosphoric acid solution, per ANSI and National Sanitation Foundation), http://mauiwater.org/phosphates.html	Terminal fate product; phosphates can persist

Table 7 **Risk-Based Criteria for the Initial Priority Chemicals and Their Key Transformation Products in Water**

Chemical	CAS RN	Water Concn *(µg/L)*	Basis	Citation/Link for Risk-Based Value	Fate Notes
Mustard, sulfur (agents H and HD [distilled H])	505-60-2	0.25	Estimated RfDe, 0.000007 mg/kg-d (Opresko et al./Army)	Opresko et al. 2001. Chemical Warfare Agents: Current Status of Oral Reference Doses. Rev Environ Contam Toxicol 172:65-85 *estimated RfD*; the intermediate MRL of 0.07 µg/kg-d, is 10x higher *(2003)*, from ATSDR 2005, http://www.atsdr.cdc.gov/mrls.html	Hydrolysis half-life is 4–8 min at 25°C in distilled water, decreases with increasing temperature, is limited by slow dissolution rate and a freezing point of 14°C; volatilization half-life is 2–20 d
Thiodiglycol (TDG)	*111-48-8*	*14,000*	RfD, 400 ug/kg-d (Reddy et al. 2005 and Talmage et al., 2007)	Reddy, G, AA Major and GJ Leach. 2005. Toxicity Assessment of Thiodiglycol. Internat. J. Toxicol. 24:435–442; Talmage et al. (2007). The Fate of Chemical Warfare Agents in the Environment, p. 89–125, as cited in TC Marrs, RL Maynard and F Sidell (eds.) *Chemical Warfare Agents: Toxicology and Treatment* (2nd Edition), http://www.wiley.com/WileyCDA/WileyTitle/productCd-0470013591.html.	Primary hydrolysis product of H (via hemisulfur mustard intermediate), along with HCl; hydrolysis half-life is 6 wk
Mustard sulfoxide	*5819-08-9*	*(0.25)*	Protectively represented by estimate RfD for the parent H, 0.000007 mg/kg-d (Opresko et al./Army)	Opresko et al. 2001 (as for sulfur mustard above), http://www.ncbi.nlm.nih.gov/entrez/query.fcgi?cmd=Retrieve&db=PubMed&list_uids=9597943&dopt=Abstract (moderately toxic, rat/mouse acute toxicity lower than H)	Oxidation product, notably in water with chlorine/hypochlorite, persists at least 1–2 d; resists hydrolysis in natural systems
Mustard sulfone	*471-03-4*	*(0.25)*	Protectively represented by estimated RfD for the parent H, 0.000007 mg/kg-d (Opresko et al./Army)	Opresko et al. 2001 (as for sulfur mustard above), http://www.ncbi.nlm.nih.gov/entrez/query.fcgi?cmd=Retrieve&db=pubmed&dopt=Abstract&list_uids=9597943&query_hl=1 (the sulfoxide is moderately toxic, with rat and mouse acute toxicity lower than for H)	Formed by further oxidation of mustard sulfoxide under more severe conditions; persistence is as for the sulfoxide, at least 1–2 d in highly oxidizing conditions
Divinyl sulfone	*77-77-0*	*(0.25)*	Protectively represented by the estimated RfD for H above, 0.000007 mg/kg-d (Opresko et al./Army)	Opresko et al. 2001 (as above), http://www.ncbi.nlm.nih.gov/entrez/query.fcgi?cmd=Retrieve&db=pubmed&dopt=Abstract&list_uids=9597943&query_hl=1 (rat oral LD_{50} is half that for H)	Product of mustard sulfone dehydrochlorination in weakly alkaline solution; volatilizes from surface water, half-life 1–10 d
Mustard, sulfur, distilled, with T (agent HT: Mixture of 60% HD, 40% T) *(same 4 fate products as H, repeat from above)*	Agent T = CAS 6392-89-8; Agent HD = CAS 505-60-2	0.25	Estimated RfD, 0.000007 mg/kg-d (Opresko et al./CDC)	Opresko et al. 2001; CDC 2004, http://www.cdc.gov/nceh/demil/files/Federal%20Register%20Mustard%20AEL%205_2004.pdf: CDC (2004) points out that "… toxicity data for T are inadequate for setting exposure limits. … For sulfur mustard and T mixtures, … monitoring for sulfur mustard alone should be sufficient under most circumstances to prevent exposure to it."	For largest fraction (60%), same fate as for H; see entries above for TDG, sulfoxide, and sulfones; T hydrolyzes to other compounds for which no applicable chronic public benchmarks were found

Table 7 Risk-Based Criteria for the Initial Priority Chemicals and Their Key Transformation Products in Water

Chemical	CAS RN	Water Concn. *(µg/L)*	Basis	Citation/Link for Risk-Based Value	Fate Notes
Nicotine	54-11-5	(70)	Intake-adjusted from 2 ppm tolerance for food residues (EPA OPPTS)	EPA 2002c (40 CFR 180.167; cucumber, lettuce, tomato), http://frwebgate.access.gpo.gov/cgi-bin/get-cfr.cgi?YEAR=2002&TITLE=40&PART=180&SECTION=167&SUBPART=&TYPE=TEXT indicator using 52 g/d per capita intakes (assumed taken in within 2 L ingested), from EPA 1997a, (Tables 9–25) http://cfpub.epa.gov/ncea/cfm/recordisplay.cfm?deid=12464	Miscible in water but not expected to hydrolyze (main change is from biodegradation)
Phorate (Thimet)	298-02-2	7	RfD, 0.0002 mg/kg-d (EPA HEAST)	EPA (2007a) RfD on HEAST, http://epa-heast.ornl.gov/Phorate.shtml; also DWLOC for child (chronic) in EPA 2001 (for the most sensitive group, child age 1–6), http://www.epa.gov/oppsrrd1/REDs/phorate_ired.pdf; note the OPP RfD of 0.0005 mg/kg-d would give 18 µg/L, EPA 1999c *(Human Health Risk Assessment: Phorate)*, http://www.epa.gov/pesticides/reregistration/phorate/; chronic population-adjusted dose gives 6 µg/L	Oxidizes to the sulfoxide and sulfone; hydrolysis half-life is 3–61 d; forms diethyldisulfide, formaldehyde and hydrogen sulfide; volatilization half life is 2–15 wk
Phorate sulfoxide	*2588-03-6*	*6*	RfD, 0.00017 mg/kg-d (EPA OPP)	EPA 1998b; http://www.ecologic-ipm.com/PDP/Table3_1998.pdf	Oxidation product; more persistent than the phorate parent
Phorate sulfone	*2588-04-7*	*6*	RfD, 0.00017 mg/kg-d (EPA OPP)	EPA 1998b; http://www.ecologic-ipm.com/PDP/Table3_1998.pdf	Oxidation product, more persistent than the phorate parent
Hydrogen sulfide (H_2S)	*7783-06-4*	*200*	Suggested drinking water limit based on health effects, 0.2 ppm (MDCH)	Michigan Department of Community Health (MDCH) (undated, accessed 2006), drinking water limit, http://www.michigan.gov/documents/hydrogensulfide_factsheet_6538_7.pdf (note that the EPA RfD of 0.003 mg/kg-d that had translated to 105 µg/L was withdrawn in 2003, http://www.epa.gov/IRIS/subst/0061.htm)	Hydrolysis product, oxidizes to the sulfate; hydrolysis half-life is 50 d at 25°C and pH 8
Hydrogen sulfate (H_2SO_4) *as sulfate (CAS 14808 79 8)*	*7664-93-9*	*250,000*	SMCL for Sulfate, 250 mg/L (EPA Office of Water)	EPA 2004a, http://www.epa.gov/waterscience/criteria/drinking/standards/dwstandards.pdf, listed in the Drinking Water Advisory Table	Terminal product, sulfate can persist
Formaldehyde	*50-00-0*	*7,000*	RfD, 0.2 mg/kg-d (EPA IRIS)	EPA *(1990)*, http://www.epa.gov/iris/subst/0419.htm; this is also the DWEL and the 1999 MRL; the 1993 *draft* HA is 1 mg/L, or 1,000 µg/L (EPA 2004a)	Hydrolysis product, can oxidize slowly to formic acid, converts to paraformaldehyde and polymers (can biodegrade in a few days)
Sarin (agent GB)	107-44-8	0.7	Estimated RfD, 0.00002 mg/kg-d (Army, Opresko et al 2001)	Opresko et al. 2001 (same reference as for Lewisite)	Hydrolysis half-life is 24 h at 25°C and pH 7.5, faster at higher pH; forms HF and IMPA, then MPA and isopropanol; does not volatilize from water

Table 7 **Risk-Based Criteria for the Initial Priority Chemicals and Their Key Transformation Products in Water** *(Set 1)*[a]

Chemical	CAS RN	Water Concn. *(µg/L)*	Basis	Citation/Link for Risk-Based Value	Fate Notes
Hydrofluoric acid, HF, as F	*7664-39-3*	*4,000*	MCL, 4 mg/L (EPA Office of Water) (for Fluoride)	EPA 2004a, MCL is 4 mg/L or 4,000 ug/L, http://www.epa.gov/safewater/contaminants/index.html; IRIS RfD of 0.06 mg/kg-d, EPA *(1989)*, http://www.epa.gov/iris/subst/0053.htm, for soluble F; more recent non-EPA value is lower, MRL 0.05 mg/kg-d, for Sodium Fluoride, 1,800 µg/L, ATSDR 2003a, http://www.atsdr.cdc.gov/toxprofiles/tp11-c2.pdf; Cal/EPA2005b, RfD 0.04 mg/kg-d is 1,400 µg/L, http://www.arb.ca.gov/toxics/healthval/contable.pdf	Primary hydrolysis product of GB; can form fluoride salts that can persist, as well as an ion pair that is unique to HF $(F^-H^+\text{-}OH_2)$
Isopropyl methylphosphonic acid (IMPA)	*1832-54-8*	*3,500*	RfD, 0.1 mg/kg-day (EPA IRIS)	EPA *(1993)*, http://www.epa.gov/iris/subst/0530.htm; Same value also referenced in: Talmage et al (2007). The Fate of Chemical Warfare Agents in the Environment, p. 89-125, as cited in TC Marrs, RL Maynard and F Sidell (eds.) *Chemical Warfare Agents: Toxicology and Treatment* (2nd Edition), http://www.wiley.com/WileyCDA/WileyTitle/productCd-0470013591.html. DWEL 4,000; 1992 HA 0.7 mg/L, 700 µg/L (EPA 2004a)	Primary hydrolysis product of GB; predicted half-life >1,900 yr
Methylphosphonic acid (MPA)	*993-13-5*	*700*	Estimated RfD, 0.020 mg/kg-d (Munro et al./Army/Talmage et al. 2007)	Munro et al. 1999 (RfD per structural similarity), http://ehp.niehs.nih.gov/members/1999/107p933-974munro/munrotab16B.GIF; Talmage et al (2007). The Fate of Chemical Warfare Agents in the Environment, p. 89–125, as cited in TC Marrs, RL Maynard and F Sidell (eds.) *Chemical Warfare Agents: Toxicology and Treatment* (2nd Edition), http://www.wiley.com/WileyCDA/WileyTitle/productCd-0470013591.html.	Hydrolysis product, forms very slowly from IMPA; chemically stable in the environment
Soman (agent GD)	96-64-0	0.14	Estimated RfD, 0.000004 mg/kg-d (Army, Opresko et al. 2001)	Opresko et al. 2001 (same reference as for lewisite)	Hydrolysis can be 5x slower than GB (e.g., half-life could be 5 d); forms HF and pinacolyl MPA; half-life for volatilization from water is 11–83 d
Hydrofluoric acid, HF, as F	*7664-39-3*	*4,000*	MCL, 4 mg/L (EPA Office of Water) (for Fluoride)	EPA 2004a, MCL is 4 mg/L or 4,000 ug/L, http://www.epa.gov/safewater/contaminants/index.html; IRIS RfD of 0.06 mg/kg-d, EPA *(1989)*, http://www.epa.gov/iris/subst/0053.htm, for soluble F; more recent non-EPA value is lower, MRL 0.05 mg/kg-d, , for Sodium Fluoride, 1,800 µg/L, ATSDR 2003a, http://www.atsdr.cdc.gov/toxprofiles/tp11-c2.pdf; Cal/EPA 2005b, RfD 0.04 mg/kg-d is 1,400 µg/L, http://www.arb.ca.gov/toxics/healthval/contable.pdf	Primary hydrolysis product of GD; can form fluoride salts that can persist, as well as an ion pair that is unique to HF $(F^-H^+\text{-}OH_2)$
Methylphosphonic acid (MPA)	*993-13-5*	*700*	Estimated RfD, 0.020 mg/kg-d (Munro et al./Army/Talmage et al. 2007)	Munro et al. 1999 (per similar chemical), http://ehp.niehs.nih.gov/members/1999/107p933-974munro/munrotab16B.GIF; Talmage et al (2007). The Fate of Chemical Warfare Agents in the Environment, p. 89–125, as cited in TC Marrs, RL Maynard and F Sidell (eds.) *Chemical Warfare Agents: Toxicology and Treatment* (2nd Edition), http://www.wiley.com/WileyCDA/WileyTitle/productCd-0470013591.html.	Hydrolysis product, forms very slowly from pinacolyl MPA; is chemically stable in environment

Table 7 Risk-Based Criteria for the Initial Priority Chemicals and Their Key Transformation Products in Water *(Set 1)*[a]

Chemical	CAS RN	Water Concn. *(µg/L)*	Basis	Citation/Link for Risk-Based Value	Fate Notes
Strychnine	57-24-9	11	RfD, 0.0003 mg/kg-d (EPA IRIS)	EPA *(1988)*, http://www.epa.gov/iris/subst/0103.htm	Poorly soluble, and essentially no hydrolysis at pH 5, 7, 9; likely removal process is adsorption
Tabun (agent GA)	77-81-6	1.4	Estimated RfD, 0.00004 mg/kg-d (Army, Opresko et al. 2001)	Opresko et al. 2001 (same reference as for lewisite)	Hydrolysis half-life is 8.5 hr at pH 7; lower in acidic, basic water
Hydrogen cyanide (HCN)	*74-90-8*	*700*	RfD, 0.02 mg/kg-day (EPA IRIS)	EPA *(1993)*, http://www.epa.gov/iris/subst/0060.htm; based on cyanide toxicity	Primary hydrolysis product; can form free CN, as well as CK with humic acid and chlorine residuals
Cyanide (CN), free	*57-12-5*	*200*	MCL, 0.2 mg/L (EPA Office of Water)	EPA *(2004a)* 1992 cyanide MCL is 0.2 mg/L, or 200 ug/L, from http://www.epa.gov/safewater/contaminants/index.html; IRIS RfD is 0.02 mg/kg-d, EPA *(1993)*, http://www.epa.gov/iris/subst/0031.htm; the RfD is for cyanide; the DWEL is 800 µg/L and lifetime HA is 200 µg/L, identified as under review in EPA 2004a (listed under cyanide with the CAS number 143-33-9 for sodium cyanide)	Most will exist as HCN (>99% at pH<7); hydrolyzes slowly to formamide, then formic acid and ammonia; much will volatilize at pH <9.2, with half-lives of 22 and 110 hr for 25 and 200 µg/L, respectively
Ammonia (NH_3) (same 2 fate products as shown for chloropicrin: nitrate and nitrite; repeat from above)	*7664-41-7*	*34,000*	RfD, 34 mg/L (EPA HEAST)	EPA (2007a), HEAST online database, http://epa-heast.ornl.gov/Ammonia.shtml; also there is a HA of 30 mg/L from EPA *(1992)*, lifetime HA, listed in EPA 2004a	Dissolves readily and forms the ammonium ion (microbes can convert to nitrate/nitrite, e.g., in surface waters/reservoirs; see those entries under chloropicrin above and for CK, CN in Table 8)
Phosphoric acid, phosphate	*7664-38-2*	*12,000*	Drinking water guideline, 12 ppm (Maui DOWS)	Maui DOWS 2004 (health-based level for phosphoric acid, from ANSI and National Sanitation Foundation), http://mauiwater.org/phosphates.html	Terminal product of GA hydrolysis; phosphates can persist
Tetraethyl pyrophosphate (TEPP)	107-49-3	*No specific drinking water benchmark found; this entry is included to introduce the fate product for which a benchmark exists*			Hydrolyzes to diethyl phosphate with a 7-hr half-life, then to ethanol and phosphoric acid
Phosphoric acid, phosphate	*7664-38-2*	*12,000*	Drinking water guideline, 12 ppm (Maui DOWS)	Maui DOWS 2004 (as above under HCN entry), http://mauiwater.org/phosphates.html	Terminal hydrolysis product, phosphates can persist
Trimethyl phosphite (TMP)	121-45-9	(1,500)	Represented by DMP, from oral SF per mg/kg-d (NAS)	NAS 2000a *(Organic Phosphonates, in Toxicological Risks of Selected Flame-Retardant Chemicals)*, http://www.nap.edu/books/0309070473/html/328.html	Hydrolyzes to DMP, methanol (<20 min half-life), then to MP, methanol, and phosphorous acid
Dimethyl phosphite (DMP)	*868-85-9*	*1,500*	SF, 0.0054 per mg/kg-d (NAS)	NAS 2000a (as described in main entry earlier in table), http://www.nap.edu/books/0309070473/html/328.html	Hydrolyzes to methanol, MP, phosphoric acid (see main entry)
Methanol	*67-56-1*	*18,000*	RfD, 0.5 mg/kg-d (EPA IRIS)	EPA (1993), http://www.epa.gov/iris/subst/0305.htm	Hydrolysis product of TMP, DMP, and MP; volatilization half-life is 5–52 d

Table 7 Risk-Based Criteria for the Initial Priority Chemicals and Their Key Transformation Products in Water *(Set 1)*[a]

Chemical	CAS RN	Water Concn *(µg/L)*	Basis	Citation/Link for Risk-Based Value	Fate Notes
Phosphoric acid, phosphate	*7664-38-2*	*12,000*	Drinking water guideline, 12 ppm (Maui DOWS)	Maui DOWS 2004 (as above under HCN entry), http://mauiwater.org/phosphates.html	Oxidation product of phosphorous acid; phosphates can persist
VX, or: O-ethyl-S-[2-(diisopropylamino)ethyl] methylphosphonothioate	50782-69-9	0.021	Estimated RfD, 0.0000006 mg/kg-d (Opresko et al. 2001)	Opresko et al. 2001	Dissolves rapidly; can slowly decompose through ion-catalyzed hydrolysis (to EA 2192), with a half-life of 17–42 d at pH 7, 25°C
S-[2-(diisopropylamino)ethyl] methylphosphonothioate (EA 2192)	*73207-98-4*	*0.021*	Estimated RfD, 0.0006 µg/kg-d (Munro et al./ Army/Talmage et al. 2007)	Munro et al. 1999 (per similar chemical; nearly as toxic at VX), http://ehp.niehs.nih.gov/members/1999/107p933-974munro/munrotab16B.GIF; Talmage et al (2007). The Fate of Chemical Warfare Agents in the Environment, p. 89-125, as cited in TC Marrs, RL Maynard and F Sidell (eds.) *Chemical Warfare Agents: Toxicology and Treatment* (2nd Edition), http://www.wiley.com/WileyCDA/WileyTitle/productCd-0470013591.html.	Primary hydrolysis product, about half follows this pathway in distilled water; hydrolysis half-life is >1,000 hr; is more stable than VX
Diisopropyl ethyl mercaptoamine (DESH)	*5842-07-9*	*130*	Estimated RfD, 3.8 µg/kg-d (Munro et al./ Army/Talmage et al. 2007)	Munro et al. 1999 (per similar chemical), http://ehp.niehs.nih.gov/members/1999/107p933-974munro/munrotab16B.GIF; Talmage et al (2007). The Fate of Chemical Warfare Agents in the Environment, p. 89-125, as cited in TC Marrs, RL Maynard and F Sidell (eds.) *Chemical Warfare Agents: Toxicology and Treatment* (2nd Edition), http://www.wiley.com/WileyCDA/WileyTitle/productCd-0470013591.html.	Primary hydrolysis product; in distilled water about a third follows this pathway; is more stable than VX
O-ethyl methylphosphonic acid (EMPA)	*1832-53-7*	*980*	Estimated RfD, 28 µg/kg-d (Munro et al./ Army/Talmage et al. 2007)	Munro et al. 1999 (per similar chemical), http://ehp.niehs.nih.gov/members/1999/107p933-974munro/munrotab16B.GIF; Talmage et al (2007). The Fate of Chemical Warfare Agents in the Environment, p. 89-125, as cited in TC Marrs, RL Maynard and F Sidell (eds.) *Chemical Warfare Agents: Toxicology and Treatment* (2nd Edition), http://www.wiley.com/WileyCDA/WileyTitle/productCd-0470013591.html.	Primary hydrolysis product, as for DESH; estimated hydrolysis half-life is >330,000 yr (assuming first-order kinetics)
Methylphosphonic acid (MPA)	*993-13-5*	*700*	Estimated RfD, 20 µg/kg-d (Munro et al./ Army/Talmage et al. 2007)	Munro et al. 1999 (per similar chemical), http://ehp.niehs.nih.gov/members/1999/107p933-974munro/munrotab16B.GIF; Talmage et al (2007). The Fate of Chemical Warfare Agents in the Environment, p. 89-125, as cited in TC Marrs, RL Maynard and F Sidell (eds.) *Chemical Warfare Agents: Toxicology and Treatment* (2nd Edition), http://www.wiley.com/WileyCDA/WileyTitle/productCd-0470013591.html.	Hydrolysis product forms very slowly from EMPA; MPA itself is chemically stable

Table 7 Risk-Based Criteria for the Initial Priority Chemicals and Their Key Transformation Products in Water *(Set 1)*[a]

Chemical	CAS RN	Water Concn *(μg/L)*	Basis	Citation/Link for Risk-Based Value	Fate Notes
Methylphosphonic acid (MPA)	*993-13-5*	*700*	Estimated RfD, 20 μg/kg-d (Munro et al./Army/Talmage et al. 2007)	Munro et al. 1999 (per similar chemical), http://ehp.niehs.nih.gov/members/1999/107p933-974munro/munrotab16B.GIF; Talmage et al (2007). The Fate of Chemical Warfare Agents in the Environment, p. 89-125, as cited in TC Marrs, RL Maynard and F Sidell (eds.) *Chemical Warfare Agents: Toxicology and Treatment* (2nd Edition), http://www.wiley.com/WileyCDA/WileyTitle/productCd-0470013591.html.	Hydrolysis product forms very slowly from EMPA; MPA itself is chemically stable
2-Diisopropylaminoethanol	*96-80-0*	*290*	Estimated RfD, 8.4 μg/kg-d (Munro et al./Army/Talmage et al. 2007)	Munro et al. 1999 (per similar chemical), http://ehp.niehs.nih.gov/members/1999/107p933-974munro/munrotab16B.GIF; Talmage et al (2007). The Fate of Chemical Warfare Agents in the Environment, p. 89-125, as cited in TC Marrs, RL Maynard and F Sidell (eds.) *Chemical Warfare Agents: Toxicology and Treatment* (2nd Edition), http://www.wiley.com/WileyCDA/WileyTitle/productCd-0470013591.html.	Primary hydrolysis product of VX, stability expected to be similar to DESH
O-ethylmethylphosphonothioic acid (EMPTA)	*18005-40-8*	*250*	Estimated RfD, 7 μg/kg-d (Munro et al./Army/Talmage et al. 2007)	Munro et al. 1999 (per similar chemical), http://ehp.niehs.nih.gov/members/1999/107p933-974munro/munrotab16B.GIF; Talmage et al. (2007). The Fate of Chemical Warfare Agents in the Environment, p. 89–125, as cited in TC Marrs, RL Maynard and F Sidell (eds.) *Chemical Warfare Agents: Toxicology and Treatment* (2nd Edition), http://www.wiley.com/WileyCDA/WileyTitle/productCd-0470013591.html.	Primary hydrolysis product of VX, stability expected to be similar to DESH

[a] This table summarizes risk-based criteria relevant to the 23 initial priority chemicals and their key transformation products (indented in italics), including fate products repeated for several threat contaminants. Two of the primary chemicals — ED and TEPP — are represented by fate products, and the value for a third (nicotine) was derived from an oral benchmark for residues. Some fate products are common to more than one threat contaminant, while other concentrations are unique.

Parentheses indicate values determined from other chemicals, including as scaled from parent compounds. Calculated values are rounded to two significant figures.

Unless otherwise noted, concentrations represent limits for long-term exposures. EPA benchmarks are prioritized, with others included as further context; lower values shown in lighter font (green). For chemicals with both a cancer and noncancer toxicity value in IRIS for a given route, the lower corresponding concentration is used. For example, the arsenic RfD of 0.0003 mg/kg-d translates to 10.5 μg/L (rounded to 11), while the concentration corresponding to the 10^{-6} risk level is lower (0.02 μg/L), so that value is listed above. Limits based only on aesthetics and not health are not presented here (e.g., secondary maximum contaminant levels based on taste, such as 250,000 μg/L for chloride, which would have applied to the common fate product hydrogen chloride if it were health-based).

For hydrogen sulfide, 0.2 ppm is the limit suggested by the State of Michigan based on health effects (from MDCH, accessed 2006). Note for TEPP, the value based on a preliminary internal evaluation of limited data could be somewhat below 9 μg/L. For nicotine, the 2 ppm tolerance for residue on cucumbers, lettuce, and tomatoes was combined with information on the average intakes of these foods (52 g/d, from 5.2, 16.3, and 30.2 g/d, respectively; EPA 1997a). Assuming no hydrolysis, scaling this amount to an ingestion rate of 2 L/d would translate to 52 μg/L as a possible indicator (to be refined in further evaluations, e.g., to also consider relative oral bioavailability).

Table 8 **Risk-Based Criteria for Additional Chemical Agents and Their Key Transformation Products in Water**

Chemical	CAS RN	Water Concn. *(µg/L)*	Basis	Citation/Link for Risk-Based Value	Fate Notes
Arsine (agent SA)	7784-42-1	*No specific drinking water benchmark found; converts quickly in water; this entry is included to introduce the fate product for which a benchmark exists*			Hydrolyzes rapidly in light, to elemental arsenic; oxidizes to arsenite, arsenate (note that in the dark with no air at 15.5 °C, 1/3 hydrolyzes within 5 hr and 2/3 within 1 d)
Arsenic (inorganic)	*7440-38-2*	*10*	MCL, 0.01 mg/L (EPA Office of Water)	EPA *(2004a)*,The MCL is 10 ug/L (from 50 ug/L in 2001), http://www.epa.gov/safewater/contaminants/index.html, as is the DWEL; the IRIS DWUR is 0.00005 per ug/L, 0.02ug/L for 10-6 risk level, EPA *(1998)*, http://www.epa.gov/iris/subst/0278.htm; 1993 RfD of 0.0003 mg/kg-d *(also 2000 Cal/EPA, 1995 draft HA, 2005 MRL)* gives 11 µg/L (rounded)	Hydrolysis products; arsenic compounds can persist for years, can settle out within months (e.g., in surface waters)
Cyanogen chloride (agent CK)	506-77-4	1,800	RfD, 0.05 mg/kg-d (EPA IRIS)	EPA *(1995a)* http://www.epa.gov/IRIS/subst/0024.htm; Additional toxicity values include 0.03 mg/kg-d from Opresko et al. *(1998)*, http://chppm-www.apgea.army.mil/chemicalagent/PDFFiles/Opreskoetal1998_EstimatingCWRfDs_RECT.pdf; there is also a HA RfD of 0.05 mg/kg-d, which is the same as the IRIS RfD, EPA 2004a (Drinking Water Standards and Health Advisories, under review; note DWEL is 2,000 µg/L), http://www.epa.gov/waterscience/criteria/drinking/standards/dwstandards.pdf; CHPPM RfD (ingestion) is 0.750 mg/L, or 750 µg/L, in CHPPM 1998, http://chppm-www.apgea.army.mil/dts/docs/detck.pdf	Significant hydrolysis to cyanic and hydrochloric acids, 5-hr half-life at pH 8.6, 20°C; slower in neutral to acid pH; cyanic acid hydrolyzes to CO_2 and ammonium chloride/ NH_3; note CK converts to cyanide in the body, but not via hydrolysis in water
Ammonia (NH_3)	*7664-41-7*	*34,000*	RfD, 34 mg/L (EPA HEAST)	EPA *(2007a)*, HEAST online database, http://epa-heast.ornl.gov/Ammonia.shtml; also there is a HA of 30 mg/L from EPA *(1992)* lifetime HA, EPA 2004a	Dissolves readily and forms the ammonium ion (microbes can convert to nitrate/nitrite, e.g., in surface waters/reservoirs)
Nitrate (NO_3^-), as N	*14797-55-8*	*10,000*	MCL, 10mg/L (EPA Office of Water)	EPA 2004a, 1992 MCL, 10 mg/L, http://www.epa.gov/safewater/contaminants/index.html. EPA *(1997)*, http://www.epa.gov/iris/subst/0078.htm, for 10-kg child (70-kg adult, 2 L/d, is 56,000 µg/L)	Oxidation product of ammonia, nitrogen naturally cycles in the environment
Nitrite (NO_2^-), as N	*14797-65-0*	*1,000*	MCL, 1 mg/L (EPA Office of Water)	EPA 2004a, 1992 MCL, 1 mg/L, http://www.epa.gov/safewater/contaminants/index.html. EPA *(1997)*, http://www.epa.gov/iris/subst/0078.htm, for the 10-kg child (70-kg adult, 2 L/d, would be 3,500 µg/L)	Oxidation product of ammonia, nitrogen naturally cycles in the environment

Table 8 Risk-Based Criteria for Additional Chemical Agents and Their Key Transformation Products in Water

Chemical	CAS RN	Water Concn *(µg/L)*	Basis	Citation/Link for Risk-Based Value	Fate Notes
Cyclohexyl sarin (agent GF, or cyclosarin)	329-99-7	0.14	Estimated RfD, 0.000004 µg/kg-d (Army CHPPM)	CHPPM *(2006)*, Chemical Warfare Agent Criteria, Summary Information, March 2006, http://usachppm.apgea.army.mil/chemicalagent/PDFFiles/ChemicalWarfareAgentCriteria_SummaryMar2006.pdf, GD and GF should have the same toxicity value, 4E-6 mg/kg-d.	Hydrolysis half-life 42 hr at 25°C (distilled water); forms HF and cyclohexyl MPA, then MPA and cyclohexanol (like GB)
Hydrofluoric acid, HF, as F	*7664-39-3*	*4,000*	MCL, 4 mg/L (EPA Office of Water) (for Fluoride)	EPA 2004a, MCL is 4 mg/L or 4,000 ug/L, http://www.epa.gov/safewater/contaminants/index.html; IRIS RfD of 0.06 mg/kg-d, EPA *(1989)*, http://www.epa.gov/iris/subst/0053.htm, for soluble F; a more recent non-EPA value is lower, the 2003 MRL of 0.05 mg/kg-d, for Sodium Fluoride, (gives 1,800 µg/L), in ATSDR 2005, http://www.atsdr.cdc.gov/mrllist_12_05.pdf; Cal/EPA, RfD 0.04 mg/kg-d is 1,400 µg/L, 2005b, http://www.arb.ca.gov/toxics/healthval/contable.pdf	Primary hydrolysis product of GF; can form fluoride salts that can persist, as well as an ion pair that is unique to HF $(F^{-}H^{+}\text{-}OH_2)$
Methylphosphonic acid (MPA)	*993-13-5*	*700*	Estimated RfD, 20 µg/kg-d (Army CHPPM/ Munro et al./ Talmage et al. 2007)	CHPPM *(1999)*, Suggested Interim Estimates of the Reference Dose (RfD) and Reference Concentration (RfC) for Certain Key Breakdown Products of Chemical Agents, as cited in Derivation of HBESLs for CWA, Appendix F, March 1999; Munro et al. 1999 (per similar chemical), http://ehp.niehs.nih.gov/members/1999/107p933-974munro/munrotab16B.GIF; Talmage et al *(2007)*. The Fate of Chemical Warfare Agents in the Environment, p. 89-125, as cited in TC Marrs, RL Maynard and F Sidell (eds.) Chemical Warfare Agents: Toxicology and Treatment (2nd Edition), http://www.wiley.com/WileyCDA/WileyTitle/productCd-0470013591.html.	Hydrolysis product forms very slowly from cyclohexyl MPA; chemically stable in the environment
Ethyl sarin (agent GE)	1189-87-3	(0.7)	Represented by Estimated RfD for sarin, 0.00002 mg/kg-d (Army, Opresko et al. 2001)	Opresko et al 2001 (taken to be represented by the RfD for GB	Similar to GB but somewhat slower hydrolysis; forms HF and EMPA, then MPA and ethanol (analogous to GB)
Hydrofluoric acid, HF, as F	7664-39-3	*4,000*	MCL, 4 mg/L (EPA Office of Water) (for Fluoride)	EPA 2004a, MCL is 4 mg/L or 4,000 ug/L, http://www.epa.gov/safewater/contaminants/index.html; IRIS RfD of 0.06 mg/kg-d, EPA *(1989)*, http://www.epa.gov/iris/subst/0053.htm, for soluble F; see entry under GF above (MRL of 1,800 µg/L, for Sodium Fluoride, Cal/EPA RfD gives 1,400 µg/L)	Primary hydrolysis product of GE; can form fluoride salts that can persist, and an ion pair that is unique to HF $(F^{-}H^{+}\text{-}OH_2)$

Table 8 Risk-Based Criteria for Additional Chemical Agents and Their Key Transformation Products in Water

Chemical	CAS RN	Water Concn *(µg/L)*	Basis	Citation/Link for Risk-Based Value	Fate Notes
O-ethyl methylphosphonic acid (EMPA)	*1832-53-7*	*980*	Estimated RfD, 0.028 mg/kg-d (Munro et al./ Army/Talmage et al. 2007)	Munro et al. 1999 (per similar chemical), http://ehp.niehs.nih.gov/members/1999/107p933-974munro/munrotab16B.GIF; Talmage et al. *(2007)*. The Fate of Chemical Warfare Agents in the Environment, p. 89–125, as cited in TC Marrs, RL Maynard and F Sidell (eds.) *Chemical Warfare Agents: Toxicology and Treatment* (2nd Edition), http://www.wiley.com/WileyCDA/WileyTitle/productCd-0470013591.html.	Primary hydrolysis product of GE; estimated hydrolysis half-life >330,000 yr (assuming first-order kinetics)
Methylphosphonic acid (MPA)	*993-13-5*	*700*	Estimated RfD, 0.020 mg/kg-d (Munro et al./ Army/Talmage et al. 2007)	Munro et al. 1999 (per similar chemical), http://ehp.niehs.nih.gov/members/1999/107p933-974munro/munrotab16B.GIF; Talmage et al. *(2007)*. The Fate of Chemical Warfare Agents in the Environment, p. 89–125, as cited in TC Marrs, RL Maynard and F Sidell (eds.) *Chemical Warfare Agents: Toxicology and Treatment* (2nd Edition), http://www.wiley.com/WileyCDA/WileyTitle/productCd-0470013591.html.	Hydrolysis product forms very slowly from EMPA; MPA itself is chemically stable in the environment
Hydrogen cyanide (HCN, agent AC)	74-90-8	700	RfD, 0.02 mg/kg-d (EPA IRIS)	EPA *(1993)*, http://www.epa.gov/iris/subst/0060.htm; based on cyanide toxicity	Much volatilizes at pH <9.2, half-life of 22–110 hr for solutions with 25–200 µg/L; hydrolyzes to formamide, then formic acid and ammonia; slower hydrolysis at pH <7
Cyanide (CN), free	*57-12-5*	*200*	MCL, 0.2 mg/L (EPA Office of Water)	EPA *(2004a)* 1992 cyanide MCL is 0.2 mg/L, or 200 ug/L, from http://www.epa.gov/safewater/contaminants/index.html; IRIS RfD is 0.02 mg/kg-d, EPA *(1993)* http://www.epa.gov/iris/subst/0031.htm, the RfD is for cyanide; DWEL is 800 µg/L, lifetime HA is 200 µg/L (under review per EPA 2004a; as cyanide with CAS for sodium CN)	Most will exist as HCN (>99% at pH<7); hydrolyzes slowly to formamide, then formic acid and ammonia; much will volatilize at pH <9.2, with half-lives of 22 and 110 hr for 25 and 200 µg/L, respectively
Ammonia (NH_3)	*7664-41-7*	*34,000*	RfD, 34 mg/L (EPA HEAST)	EPA *(2007a)*, HEAST online database, http://epa-heast.ornl.gov/Ammonia.shtml; also there is a HA of 30 mg/L from EPA *(1992)* lifetime HA, EPA 2004a	Dissolves readily and forms the ammonium ion (microbes can convert to nitrate/nitrite, e.g., in surface waters/reservoirs)
Nitrate (NO^-_3)*, as N*	*14797-55-8*	*10,000*	MCL, 10mg/L (EPA Office of Water)	EPA 2004a, 1992 MCL, 10 mg/L, http://www.epa.gov/safewater/contaminants/index.html. EPA *(1997)*, http://www.epa.gov/iris/subst/0078.htm, for 10-kg child (70-kg adult, 2 L/d, would be 56,000 µg/L)	Oxidation product of ammonia, nitrogen naturally cycles in the environment
Nitrite (NO_2^-)*, as N*	*14797-65-9*	*1,000*	MCL, 1 mg/L (EPA Office of Water)	EPA 2004a, 1992 MCL, 1 mg/L, http://www.epa.gov/safewater/contaminants/index.html. EPA *(1997)*, http://www.epa.gov/iris/subst/0078.htm, for the 10-kg child (70-kg adult, 2 L/d, is 3,500 µg/L)	Oxidation product of ammonia, nitrogen naturally cycles in the environment

Table 8 Risk-Based Criteria for Additional Chemical Agents and Their Key Transformation Products in Water

Chemical	CAS RN	Water Concn *(µg/L)*	Basis	Citation/Link for Risk-Based Value	Fate Notes
Perfluoroisobutylene (PFIB)	382-21-8	*No specific drinking water benchmark found; this entry is included to introduce a fate product for which a benchmark exists*			Hydrolyzes to fluorophosgene, then HF and CO_2
Hydrofluoric acid, HF, as F	*7664-39-3*	*4,000*	MCL, 4 mg/L (EPA Office of Water) (for Fluoride)	EPA 2004a, MCL is 4 mg/L or 4,000 ug/L, http://www.epa.gov/safewater/contaminants/index.html; IRIS RfD of 0.06 mg/kg-d, EPA *(1989)*, http://www.epa.gov/iris/subst/0053.htm, for soluble F; a more recent non-EPA value is lower, the MRL of 0.05 mg/kg-d, for Sodium Fluoride, gives 1,800 µg/L, ATSDR 2005a, http://www.atsdr.cdc.gov/mrllist_12_05.pdf; Cal/EPA 2005b, RfD 0.04 mg/kg-d is 1,400 µg/L, http://www.arb.ca.gov/toxics/healthval/contable.pdf	Hydrolysis product, forms rapidly from fluorophosgene; can form fluoride salts that can persist, as well as an ion pair that is unique to HF *(F^-H^+-OH_2)*
Red phosphorus (RP)	7723-14-0	(0.7)	Protectively represented by RfD for white P, 0.00002 mg/kg-d (EPA IRIS)	EPA *(1993)* (white P has the same CAS, is more toxic), http://www.epa.gov/iris/subst/0460.htm, as a conservative indicator for RP; other values for white P are the earlier 1990 HA of 0.1 µg/L, and DWEL of 0.5 µg/L (EPA 2004a); and from 1997 *intermediate* MRL in ATSDR 2005, http://atsdr.cdc.gov/mrls/pdfs/mrllist_12_06.pdf, 0.0002 mg/kg-d for white P gives 7 µg/L for that shorter duration	RP slowly disproportionates, hydrolyzes, and oxidizes; forms phosphine and phosphoric acid; reaction half-life estimated at >350 yr to >3,500 yr
Phosphine	*7803-51-2*	*11*	RfD, 0.0003 mg/kg-d (EPA IRIS)	EPA *(1993)*, http://www.epa.gov/iris/subst/0090.htm; There is also a RfD established by EPA OPP, 0.0113 mg/kg-d, according to http://www.epa.gov/fedrgstr/EPA-PEST/1999/June/Day-09/p14069.htm. Application of this RfD would yield a water concentration value of 400; therefore the IRIS RfD is the most protective value.	Product of RP reaction with water and oxygen; forms very slowly, limited by solubility
Phosphoric acid, phosphate	*7664-38-2*	*12,000*	Drinking water guideline, 12 ppm (Maui DOWS)	Maui DOWS 2004 (health-based level for phosphoric acid from ANSI and National Sanitation Foundation), http://mauiwater.org/phosphates.html	Oxidation product of RP; phosphates can persist
VG, Amiton, or: *O,O*-diethyl-*S*-[2-(diethyl-amino)ethyl] phosphorothioate	78-53-5	*No direct benchmark was found. No compound-specific toxicity information for this compound is available, so assumptions cannot be made about toxicity of Amiton relative to that of nerve agent VX. Further, the fate and degradation of of Amiton is not well characterized; as a consequence, VG fate product entries are not listed.*			Degradation and hydrolysis fate of VG is not well characterized.
VM, or: *O*-ethyl-*S*-[2-(diethylamino)ethyl] methylphosphonothioate	21770-86-5	*No direct benchmark was found. No compound-specific toxicity information for this compound is available, so assumptions cannot be made about toxicity of agent VM relative to that of nerve agent VX. Further, the fate and degradation of of agent VM is not well characterized; as a consequence, VM fate product entries are not listed.*			In the absence of specific degradation information for agent VM, fate products are not assessed.

Table 8 Risk-Based Criteria for Additional Chemical Agents and Their Key Transformation Products in Water

Chemical	CAS RN	Water Concn *(µg/L)*	Basis	Citation/Link for Risk-Based Value	Fate Notes
Vx, or: *O*-ethyl-*S*-[2-(dimethylamino) ethyl] methylphosphonothioate	20820-80-8	*No specific benchmark found.*		No compound-specific information for agent Vx is available, so an assumption cannot be made about Vx toxicity relative to that of agent VX. Based on liquid skin exposure, Vx is less toxic than VX; Vx ingestion/absorption is not readily known [Dept of Army, 2005, Potential Military Chemical/Biological Agents and Compounds, FM 3-11.9, US Dept. of Army, The Pentagon, Washington, DC (approved for public release, distribution unlimited)]. No Vx toxicity estimates are recommended at this time because data are lacking. Further, in the absence of specific degradation information for Vx, fate product entries are not listed.	In the absence of specific degradation information for agent Vx, fate products are not assessed.

[a] This table identifies risk-based chronic exposure criteria relevant to additional chemical agents and their key transformation products (indented, in italics). Some agents are represented by their fate products: arsine, and PFIB. Some fate products are common to more than one primary contaminant, while others are unique. Parentheses indicate derived concentrations, e.g., from values for other chemicals. Calculated values are rounded to two significant figures. Unless otherwise noted, concentrations represent limits for long-term exposures. EPA benchmarks are prioritized, with others included as further context; lower values are in lighter font (green).

For chemicals with both a cancer and noncancer toxicity value, the value corresponding to the lower concentration is shown.

No direct chronic public benchmarks were found for additional agents beyond those represented above: nitrogen mustard, red phosphorus, tear gas, and VE. Several convert quickly to other compounds in water, so chronic benchmarks would not be relevant. For example, tear gas can hydrolyze in minutes to 2-chlorobenzaldehyde and malononitrile (relatively toxic). Note that after being taken into the body (but not in water), tear gas is converted to cyanide and thiocyanate.

Table 9 **Risk-Based Criteria for Additional Industrial Chemicals and Products in Water and Air**

Chemical	**CAS RN**	**Water Concn.** *(μg/L)*	**Basis** *(Priority: EPA benchmark with most recent analysis; MCL, then others also indicated for context)*	**Air Concn.** *(μg/m³)*	**Basis** *(Priority: EPA benchmark with most recent analysis; others also indicated for context)*
Aldicarb (Temik)	116-06-3	35	IRIS RfD, 0.001 mg/kg-d *(1993)*; the DWEL is 40 μg/L; the MCL of 3 μg/L has been stayed		
Aldicarb sulfone (from aldicarb)	1646-88-4	35	IRIS RfD, 0.001 mg/kg-d *(1993)*; the DWEL is 40 μg/L; the MCL of 2 μg/L has been stayed		
Aldicarb sulfoxide (from aldicarb)	1646-87-3	35	RfD, 0.001 mg/kg-d (in EPA 2006d, 2006 Edition of the Drinking Water Standards and Health Advisories (Summer 2006), EPA 822-R-06-013, Office of Water, Washington, DC; http://www.epa.gov/waterscience/criteria/drinking/dwstandards.pdf) and the DWEL is 40 μg/L.		
Allyl alcohol	107-18-6	180	IRIS RfD, 0.005 mg/kg-d *(1989)*		
Asbestos (various forms)	1332-21-4	7 M f/L, *(est. 210 μg/L)*	MCL, 7 million fibers (Mf)/L (fibers >10 μm) *(1991)*; is also the HA; using qualified conversion of 30 μg/m³ per fiber (f)/mL (or 0.00003 μg/f) from IRIS *(1993)* this translates to 210 μg/L (note that EPA 2004a indicates a concentration of 7 Mf/L for 10^{-6} risk)	400 f/m³, *(est. 0.012 μg/m³)*	IRIS IUR, 0.23 per f/mL, 0.000004 f/mL for 10^{-6} risk *(1993)*; HA for 10^{-4} risk based on inhalation is 7 M f/L *(EPA 2006b)*; converting the 400 f/m³ from the IUR as indicated at left gives 0.012 μg/m³; the Cal/EPA IUR of 0.063 per μg/m³ is 0.000016 for 10^{-6} risk *(2005)*
Benzene (gasoline range organics)	71-43-2	5	MCL, 0.005 mg/L (1987); IRIS DWUR, 1–10 μg/L for 10^{-6} risk *(2000)*; IRIS RfD of 0.004 mg/kg-d gives 140 μg/L *(2003)*; DWEL is also 100 μg/L (in the 2006 Edition of the Drinking Water Standards and Health Advisories [EPA 822-R-06-013])	0.13	IRIS IUR, range 0.13 to 0.45 μg/m³ for 10^{-6} risk *(2000)*; IRIS RfC is 30 μg/m³ *(2003)*; CREL is 60 μg/m³ *(2000)*; draft MRL is 10 μg/m³, from 0.003 ppm (2005); earlier Cal/EPA IUR of 0.000029 per μg/m³ is 0.03 μg/m³ for 10^{-6} risk *(1985)*
Boric acid	10043-35-3	10,500	NRC (2000), RfD of 0.3 mg/kg-d, Toxicological Risks of Selected Flame-retardant Chemicals, National Research Council, http://books.nap.edu/openbook.php?record_id=9841&page=180; IRIS RfD, 0.2 mg/kg-d as B *(2004)* (water concentration value would be 40,000, using molecular weight conversion of 61.84 mg boric acid/10.81 mg boron, as boric acid)		
Boron trichloride *(B in water)*	10294-34-5	7,000	IRIS RfD, 0.2 mg/kg-d as B *(2004)*, water concentration is 76,000, using molecular weight conversion of 117.17 mg boron trichloride/10.81 mg boron, as B trichloride; DWEL is 7 mg/L (2006 Edition of the Drinking Water Standards and Health Advisories, http://www.epa.gov/waterscience/criteria/drinking/dwstandards.pdf)		
Boron trifluoride *(F in water)*	7637-07-2	(2,100)	IRIS RfD, 0.06 mg/kg-d F *(1989)*, water concentration is 3800, using molecular weight conversion of 67.81 mg boron trifluoride/37.00 mg fluorine, as BF_3; Cal/EPA RfD 0.04 mg/kg-d for Fluorides gives 1,400 *(http://www.arb.ca.gov/toxics/healthval/contable.pdf, 2003)*	0.7	HEAST RfC, 0.0007 mg/m3 (1986), http://epa-heast.ornl.gov/

Table 9 Risk-Based Criteria for Additional Industrial Chemicals and Products in Water and Air

Chemical	CAS RN	Water Concn. *(µg/L)*	Basis *(Priority: EPA MCL, then benchmark with most recent analysis; others also indicated for context)*	Air Concn. *(µg/m³)*	Basis *(Priority: EPA benchmark with most recent analysis; others also indicated for context)*
Bromadiolone	28772-56-7	(0.7)	OPP chronic NOEL, 0.002 mg/kg-d *(1998a)*; with inter/intraspecies factors (100), suggests indicator 0.7		
Cadmium	7440-43-9	5	MCL is 0.005 mg/L (1991), as is the lifetime HA (1987); IRIS RfD, 0.0005 mg/kg-d *(1994)*; DWEL is 20 µg/L; water concentration based on MRL would be 7 µg/L, from 0.0002 mg/kg-d *(1999)*	0.0006	IRIS IUR, 0.0018 per µg/m³ for 10^{-6} risk level, for concentrations not exceeding 6 µg/m³ *(1992)*; CREL is 0.02 µg/m³ *(2000)*
Carbofuran	1563-66-2	40	MCL, 0.04 mg/L (1991); with IRIS RfD, 0.005 mg/kg-d, the water concentration value would be 175 *(1987)*		
Carbon disulfide	75-15-0	3,500	RfD, 0.1 mg/kg-d *(1990)*	700	IRIS RfC *(1995)*; CREL is 800 µg/m³ *(2001)*; MRL of 0.3 ppm would give an air concentration value of 930 µg/m³ *(1996)*
Chlorine	7782-50-5	4000	MCL, 4 mg/L (1998), same as the lifetime HA; IRIS RfD, 0.1 mg/kg-d *(1994)*; the same RfD is listed in the OPP reregistration eligibility document (RED) *(EPA 1999)*	0.2	CREL *(2000)*
2-Chloroethanol	107-07-3		No compound-specific toxicity information for this compound is available, so assumptions cannot be made about toxicity relative to that of another compound.		
Cyanide salts as sodium salt (NaCN)	143-33-9	1,400	IRIS RfD, 0.04 mg/kg-d *(1996)* (1992 MCL for this CAS number as *free CN* is 200 µg/L, also the 1987 HA, DWEL for free CN is 800 µg/L); *intermediate* MRL 0.05 mg/kg-d would translate to a water concentration value of 1,800 µg/L (rounded) *(2006)*	9	CREL for HCN
1,2-Dichloroethane (ethylene dichloride)	107-06-2	5	MCL (1989); IRIS DWUR, 0.0000026 per µg /L as risk-specific concentration for 10^{-6} risk level *(1991)*; archived PPRTV RfD of .02 mg/kg-d (2002); the *intermediate* MRL of 0.2 mg/kg-d would give a water concentration value of 7,000 µg/L *(2001)*	0.04	IRIS IUR, 0.000026 per µg/m³ for 10^{-6} risk *(1991);* CREL 400 µg/m³ *(2001)*; prior Cal/EPA IUR 0.000021 per µg/m³ is 0.05 µg/m³ at 10^{-6} *(1985)*; MRL is 0.6 ppm or 2,400 µg/m³ *(2001)*
Diesel engine exhaust (mixture)	(9-91-1)		Values exist for various constituents but not the mixture	5	IRIS RfC *(2003)*, no CAS; same CREL for CAS shown (as particulates); Cal/EPA IUR, of 0.003 per µg/m³ is 0.33 µg/m³ at 10^{-4} *(1998)*
1,2-Diisopropyl methylphosphonate (DIMP)	1445-75-6	2,800	IRIS RfD 0.08 mg/kg-d *(1993)*; DWEL is 3,000; the water concentration value for the MRL of 0.6 mg/kg-d would be 21,000 µg/L *(1998)*; HA, 600 µg/L *(1989)*		
1,4-Dithiane (diethylene disulfide)	505-29-3	350	IRIS RfD, 0.01 mg/kg-d *(1993)*; DWEL is 400 µg/L; HA is 80 µg/L *(1992)*		

Table 9 Risk-Based Criteria for Additional Industrial Chemicals and Products in Water and Air

Chemical	CAS RN	Water Concn. *(µg/L)*	Basis *(Priority: EPA MCL, then benchmark with most recent analysis; others also indicated for context)*	Air Concn. *(µg/m^3)*	Basis *(Priority: EPA benchmark with most recent analysis; others also indicated for context)*
Ethylbenzene (gasoline range organics)	100-41-4	700	MCL *(1992),* also the HA *(1987)*; IRIS RfD of 0.1 mg/kg-d would give a water concentration value of 3,500 µg/L *(1991)*; DWEL is 3,000 µg/L	1,000	IRIS RfC *(1991)*; CREL is 2,000 µg/m^3; *int.* MRL is 4,300 *(1999)*
Ethylene glycol (from ethylene oxide)	107-21-1	70,000	IRIS RfD, 2 mg/kg-d *(1989; also the 1997 MRL)*; DWEL is also 70,000; while HA is 14,000 µg/L *(1987)*	400	CREL *(2000)*
Ethylene oxide (Oxirane)	75-21-8	8	HEAST oral SF of 1.02 per mg/kg-d *(1985)*	30	CREL *(2001)*; *intermediate* MRL of 0.09 ppm is 160 µg/m^3 *(1990)*; earlier Cal/EPA IUR of 0.000088 per µg/m^3 is 1.1 µg/m^3 at 10^{-4} risk *(1987)*
Fluorine *(as F$^-$ in water, HF in air)*	7782-41-4	4,000	MCL is 4 mg/L as Fluoride (1986); IRIS RfD, 0.06 mg/kg-d *(1989)* using Fluoride data; MRL of 0.05 mg/kg-d for Sodium Fluoride would give a water concentration value of 1,800 µg/L *(2003)*; the Cal/EPA RfD of 0.04 mg/kg-d for Fluorides would give a water concentration value of 1,400 µg/L *(2003)*	(14)	CREL for HF is 14 µg/m^3, 13 µg/m^3 as F$^-$ *(2003)*
Furan	110-00-9	35	IRIS RfD, 0.001 mg/kg-d *(1989)*		
Gasoline (in air: as vapors) (in water: see representative chemicals)	1-11-0		See 5 example constituents: BTEX and n-hexane	2,100	CREL *(1991)*; WI-suggested 6 ppm for homes (per work level) *(Wisconsin Department of Health and Family Services [WIDHFS] 2004)* or 18,000–27,000 µg/m^3
n-Hexane (gasoline range organics)	110-54-3	2,100	HEAST RfD of 0.06 mg/kg-d *(1989)*; the provisional RfD from EPA is also 0.06 mg/kg-d (www.epa.gov/ttn/hlthef/hexane.html); HA of 4000 µg/L *(1987)* (only as a *10-d* HA, for a 10-kg child, 1 L/d)	700	IRIS RfC *(2005)*; MRL of 0.6 ppm is 2,100 µg/m^3 *(1999)*; CREL 7,000 *(2005)*
Kerosene (C_9 to C_{16} hydrocarbons)	8008-20-6		Values exist for various constituents but not the mixture	10	MRL, *intermediate* (for 15–364 d of exposure) *(1995)*
Mercuric chloride, as mercury	7487-94-7	11	IRIS RfD, 0.0003 mg/kg-d *(1995)*; *int.* MRL 0.002 mg/kg-d would yield a water concentration value of 70 µg/L *(1999)*; DWEL of 10 µg/L for Hg; MCL of 2 µg/L for Hg (inorganic) *(1992; also 1987 HA)*	0.09	CREL, for inorganic Hg *(2000)*; *intermediate* MRL for mercury is 0.2 µg/m^3 *(1999)*
Methyl isocyanate	624-83-9		Forms methylamine, CO_2, others; no public benchmark	1	CREL *(2005)*
Oxamyl (Vydate)	23135-22-0	200	MCL *(1994)*; HA of 10 µg/L, child, 1 d and 10 d *(2005)*; IRIS RfD 0.025 mg/kg-d would yield a water concentration value of 880 µg/L *(1991)*; DWEL is 35 µg/L; of 0.001 mg/kg-d gives a water concentration value of 35 µg/L OPPTS chronic RfD*(EPA 2000d)*		
Paraquat (dichloride form)	1910-42-5	160	IRIS RfD, 0.0045 mg/kg-d *(1991)*; DWEL is 200	(0.01)	OPPTS*(1997c)* indicates *short-term* inhalation NOEL 0.01 µg/L; UF 1,000 suggests indicator of 0.01 µg/m^3

Table 9 Risk-Based Criteria for Additional Industrial Chemicals and Products in Water and Air

Chemical	CAS RN	Water Concn. *(µg/L)*	Basis *(Priority: EPA MCL, then benchmark with most recent analysis; others also indicated for context)*	Air Concn. *(µg/m³)*	Basis *(Priority: EPA benchmark with most recent analysis; others also indicated for context)*
Phenol	108-95-2	11,000	IRIS RfD, 0.3 mg/kg-d *(2002)*; this is also the DWEL; the draft HA is 2,000 µg/L *(1992)*	200	CREL *(2000)*
Polychlorinated biphenyls (PCBs)	1336-36-3	0.5	MCL *(1992)*; IRIS DWUR of 0.1 µg/L, 10^{-6} risk, if ≤1,000 µg/L *(1997)*; water concentration value for MRL is 0.7 µg/L, from 0.02 µg/kg-d Aroclor 1254 *(2000)*; Cal/EPA RfD of 0.02 µg/kg-d would give a water concentration value of 0.7 µg/L *(1996)*	0.01	IRIS IUR-based level for 10^{-6} risk, when <100 µg/m³ *(1997)*; CREL 1.2 µg/m³, while Cal/EPA IUR of 0.00057 per µg/m³ is 0.0018 µg/m³ for 10^{-6} risk *(1991)*
Propylene oxide	75-56-9	0.1	IRIS DWUR, 10^{-6} risk *(1994)*, IRIS oral SF is 0.24 per mg/kg-d; OPPTS RfD of 0.001 mg/kg-d would give a water concentration value of 35 µg/L *(see EPA 2005c)*	0.3	IRIS IUR, *(1994)*; IRIS RfC of 30 µg/m³ *(1990)*; CREL of 30 µg/m³ *(2000)*; prior Cal/EPA IUR is 3.7E-6, 27 µg/m³ for 10^{-6} risk *(1999)*
Sodium fluoroacetate (the example salt)	62-74-8	0.7	IRIS RfD, 0.00002 mg/kg-d *(1993)*, same for OPP *(1995)*		
Sulfur dioxide	7446-09-5	(500,000)	EPA *(2006b)* health-based value, 2006 Edition of the Drinking Water Standards and Health Advisories table, http://www.epa.gov/waterscience/criteria/drinking/dwstandards.pdf (For SO_4 that would form in water)	79	NAAQS, 0.03 ppm *(1990, an. av)*; CREL 660 *(1992)*
Toluene (gasoline range organics)	108-88-3	1,000	MCL(1992); IRIS RfD of 0.08 mg/kg-d *(2005)*; DWEL is 3000 µg/L	5,000	IRIS RfC *(2005)*; MRL 0.08 ppm (2000) is the CREL, 300 µg/m³ *(2000)*
Xylenes (gasoline range organics)	1330-20-7	10,000	MCL (1992); IRIS RfD, 0.2 mg/kg-d *(2003)*; DWEL (7,000 µg/L); the draft MRL, 0.6 mg/kg-d, would yield a water concentration value of 21,000 µg/L *(2005)*	100	IRIS RfC *(2003)*; MRL 0.05 ppm is 650 µg/m³ *(2005)*; the CREL is 700 µg/m³ *(2000)*

[a] This table identifies risk-based chronic exposure criteria in water and air for industrial contaminants, including four mixtures and several fate products. A number of NHSRC list chemicals are fate products of others addressed in other tables within this document, so those are not repeated here (see Table 2 note). Fate products of chemicals are italicized in this list, with parents in parentheses. Chemicals only from the SAM report (not on the NHSRC list or their fate products) are in lighter font (blue). More than half (23) have values for both air and water. Note for sulfur dioxide in air, *an. av* represents annual average.

The toxicity value dates indicate when the value was established, reassessed, or updated. The EPA sources include: IRIS (accessed 2007), MCL list (2006 table), drinking water advisories including HAs (2006 tables), NAAQS (2005 list, from 1990 and updates), and OPPTS (which includes various studies from the OPP, and Office of Pollution Prevention and Toxics, OPPT); non-EPA sources include: ATSDR: MRLs (2006 list); NZ maximum residue limit (MResL) Food Standards Australia New Zealand (FSANZ); and states, including Cal/EPA: CREL, AREL, IUR, RfD (2005a, b, c, d); and Wisconsin and Michigan limits for air and water (WIDHFS 2004, MDCH 2006).

Concentrations from a UR or SF correspond to a risk of 10^{-6}. Calculated values are rounded to 2 significant figures (e.g., for mercuric chloride and paraquat in water, and SO_2 in air). Note for ATSDR MRLs, intmd = intermediate (benchmarks for shorter durations such as intermediate MRLs that cover exposures of 15–364 days can be useful, considering discrete releases to dynamic systems, especially for nonpersistent chemicals). Parentheses are used to identify values that are (1) from draft benchmarks; (2) derived from related benchmarks, including for fate products or surrogates; and (3) from benchmarks for shorter durations, when no applicable chronic limits were found—such as the intermediate MRLs and the 10-d child HA for n-hexane.

For water values, the MCL is the priority source while IRIS is the primary source for air values. Where multiple benchmarks exist, others are also shown to offer further context for framing the method validation (for example, if a release occurred in California, Cal/EPA values would also likely be addressed). Values reflecting the most recent evaluation are preferred, and final values are preferred over drafts or those under review. As an example, although the EPA HA for boron (600 µg/L) is less than one-tenth the concentration calculated from the IRIS RfD, that RfD is from 2004 while the HA is from a 1992 draft document that is under review. When a non-EPA benchmark is lower than an EPA value, those other values are indicated in lighter font (green). For example, the concentration identified as both the MRL and Cal/EPA CREL for toluene (300 µg/m³) is about 17 times lower than the EPA RfC, but they were established in 2000 while the RfC is from 2005.

For aldicarb and its sulfoxide and sulfone, the 1995 health advisories (given in EPA 2006) indicate that the combined concentration should not exceed 7 µg/L, but the MCLs reflected in that statement (3, 4, and 2 µg/L, respectively) have been stayed. For ammonia, no health-based benchmark was found. The EPA (2005c) considers the taste threshold of about 35,000 µg/L a conservative (low) surrogate for a health-based level because it is below the NOAEL.

For asbestos, the1993 IRIS IUR is based on phase contrast microscopy (PCM) counts for fibrous material, not asbestos-specific; the correlation between PCM data and specific fiber (f) count or mass measurements by transmission electron micrsoscopy (TEM) is described as very poor. Although a conversion factor of 30 µg/m^3 per f/mL was adopted (same as Cal/EPA conversion of 100 PCM f/0.003 µg, 0.00003 µg/f), IRIS acknowledges this is highly uncertain (www.epa.gov/iris/subst/0371.htm); the Cal/EPA (2005d) IUR is 0.063 per µg/m^3, and the potency factor is 220 per mg/kg-d.

For boron trichloride in water, the toxicity of boric acid as boron (CAS 7440-42-8) is limiting. In contrast, for boron trifluoride in water the fluoride is limiting. Analytical methods for water are often based on boron equivalents, so that is the main concentration provided; molecular-weight-scaled concentrations are also provided for the full compound (molecular weight for boron is 11). Note that the earlier OPP RED report indicated an RfD of 0.09 mg/kg-d, which would be 3,200 µg/L (EPA 1994).

For bromadiolone, the indicator of 0.7 µg/L is derived from the OPP chronic level. For comparison, the New Zealand MResL is 0.001 mg/kg (noted as being set at or about the analytical quantification limit). As a crop rodenticide, considering the mean per capita U.S. intakes of vegetables (4.3), fruit (3.4), and grain (4.1), which total 11.8 g/kg-d (EPA 1997a): if the residue were at its limit, a 70-kg adult would take in 0.8 µg/d; if that amount were taken in from 2 L water instead, the equivalent concentration would be 0.4 µg/L.

Cyanide salts are conservatively represented by sodium cyanide because it is most toxic (its IRIS RfD is lowest); the range across various salts extends to 1,000 µg/L, as molecular-weight-scaled from the CN value. Note that the molecular weight ratio of NaCN/CN is 49/26 (1.9) and the NaCN RfD is double that for CN and HCN, 0.02 mg/kg-d, which correspond to 700 µg/L. The 1987 HA for cyanide is 0.2 mg/L (listed with the sodium cyanide CAS number). (Note that the current MCL from 1992 for free cyanide is 0.2 mg/L or 200 µg/L; for context, typically only about 10% of HCN in water is as free cyanide.)

Diesel exhaust constituents include polycyclic aromatic hydrocarbons (PAHs), nitrogen oxides, and particulates, such as carbon black. For gasoline range organics, automotive gasoline contains up to 150 chemicals, including the five listed above (ATSDR 1995): benzene (comprising 2%), toluene, ethylbenzene, and xylenes (BTEX), and n-hexane. The odor threshold is 0.25 ppm, and a state-recommended limit for air in homes is 6 ppm (WIDHFS 2000); with a conversion of 3-4.5 mg/m^3 (see Table A2 notes), that is 18,000-27,000 µg/m^3.

For propylene oxide, the OPP chronic oral RfD of 0.001 mg/kg-d could indicate 35 µg/L, depending on bioavailability (EPA 2005c).

Non-EPA sources include: New Zealand Food Authority (ETO and 2-chloroethanol in water), State of Michigan (H_2S in water), ATSDR (ammonia, ETO, kerosene, mercury in air), and Cal/EPA (chlorine, ethylene oxide, fluorine, HF, methyl isocyanate, and phenol). Applicable chronic public benchmarks were not found for 21 chemicals from NHSRC and SAM (see Table 12 footnote).

Information for radionuclides is provided in:

- Table 10 – Nuclear Decay Data for Primary Radionuclides and Potentially Important Radioactive Progeny (Set 4)
- Table 11 – Risk-Based Criteria for Primary Radionuclides in Water and Air (Set 4)

The persistence of radionuclides in water and air is determined by environmental processes and by the rate of physical decay of the radionuclides to stable elements or to other radionuclides. The decaying radionuclide is referred to as the parent radionuclide. A radionuclide that arises from physical decay of a parent radionuclide is referred to as a daughter radionuclide or radioactive progeny. A parent radionuclide together with a series of radioactive progeny originating with the parent is referred to as a decay chain.

The rate of physical decay of a radionuclide is described by its half-life, which is the length of time for a given amount of a radionuclide to decrease to half that amount. The amount of a radionuclide present in a given volume of material is typically measured in terms of activity, defined as the number of physical decays of the radionuclide per unit time. The International System of Units (SI) unit of activity is the becquerel (Bq), defined as one disintegration per second. In this report, activity is given in conventional units of curie (Ci) or picocurie (pCi) because these units are still commonly used in the US. SI and conventional units for activity are related as follows: 1 Ci $\sim 3.7 \times 10^{10}$ Bq, 1 pCi = 10^{-12} Ci, and 1 Bq $\sim$ 27 pCi.

Basic nuclear decay data for the 15 primary radionuclides addressed in this report and their potentially important radioactive progeny are summarized in Table 10. The listed data include half-lives, decay modes, and energies of different types of radiation emissions. Radiation energies listed for a radionuclide include its total alpha energy (if any), the prominent alpha energy and its yield (i.e., the percentage of decays of the radionuclide giving rise to the prominent alpha energy), the total photon energy (if any), the prominent photon energy and its yield, and the total energy of electron emissions. The total energy of electron emissions represents the sum of the continuous electron spectrum (beta spectrum) and discrete mono-energetic electrons.

The specific activity (activity per unit mass) of each of the 15 primary radionuclides is listed in Table 11 in units of curies per gram (Ci/g). These specific activities were used to convert risk-based activity criteria (columns 3 and 5 of Table 11) to risk-based mass criteria (columns 4 and 6, respectively). As discussed below, the specific activity indicated for uranium-238 represents a mixture of uranium-238, uranium-235 and uranium-234.

Risk-based activity criteria for water and air were based on risk coefficients given in Federal Guidance Report No. 13 (FGR 13), "Cancer Risk Coefficients for Environmental Exposure to Radionuclides" (EPA 1999). A risk coefficient for ingestion or inhalation of a radionuclide is an estimate of the probability of radiogenic cancer mortality (or morbidity) per unit activity (Bq^{-1}) of that radionuclide taken into the body. The risk coefficients in FGR13 were derived for a hypothetical stationary population whose demographics, cancer rates, and age- and gender-specific usage of environmental media other than air were based on data for the U.S. population circa 1990 (Ershow and Cantor 1989; NCHS 1992, 1993a, 1993b, 1997; McDowell et al. 1994). Age- and gender-specific air intake rates were based on reference values recommended by the International Commission on Radiological Protection (ICRP 1994).

For each of the 15 primary radionuclides addressed in the present report, separate risk coefficients for inhalation are provided in FGR 13 for different "absorption types" as defined by the ICRP (1994). An absorption type for a radionuclide carried in air as a particulate aerosol represents a specified level of solubility of the aerosol in the respiratory tract and an associated rate of absorption of the carried radionuclide to blood. The following absorption types are defined in ICRP Publication 66 (1994) and addressed in FGR 13:

- Type F, representing fast dissolution and a high level of absorption to blood;
- Type M, representing a moderate rate of dissolution and an intermediate level of absorption to blood; and
- Type S, representing slow dissolution and a low level of absorption to blood.

In many cases a default absorption type and hence a default risk coefficient for inhalation of a given radionuclide is indicated in FGR 13 for use when no information is available on the physical or chemical form of the inhaled material. The default type for a radionuclide is based on recommendations given in ICRP Publication 72 (ICRP, 1996), which reflect available information on the solubility of commonly encountered forms of the radionuclide. In the present report, the risk-based criterion for a radionuclide in air is based on its default risk coefficient if a default value is indicated in FGR 13. In each of the remaining cases (identified in footnote d to Table 11), the risk-based criterion for air is based on the maximum of the risk coefficients for inhalation of Type F, Type M, and Type S material.

Separate risk coefficients are provided in FGR 13 for ingestion of inorganic and organic forms of polonium-210 in tap water. The risk coefficient for inorganic polonium-210 was used to derive a risk-based criterion for polonium-210 in water because this is presumed to be the more likely form of this radionuclide in drinking water.

Use of a risk coefficient to derive a risk-based criterion for a radionuclide requires a reference risk, i.e., a limiting value for the projected cancer mortality risk resulting from intake of the radionuclide in water or air. For the purpose of deriving Risk-Based Criteria for radionuclides in water and air, a reference risk was chosen for consistency with excess cancer mortality risks implied by current EPA standards for radionuclides in water or air. Current standards for drinking water (EPA 2006) include a concentration limit of 15 pCi L^{-1} for alpha emitters, an annual dose limit for beta and photon emitters of 4 mrem to the total body or any organ, a concentration limit of 5 pCi L^{-1} for radium-226 and radium-228 combined, a concentration limit of 8 pCi L^{-1} for Sr-90, and a concentration limit of 30 µg L^{-1} for uranium. EPA National Emission Standards for Hazardous Air Pollutants (NESHAPs) specify an annual dose limit of 10 mrem effective dose equivalent for any member of the public from emissions of radionuclides to the ambient air (EPA 1991, 2004). These standards for water and air were developed over a period of decades for regulatory purposes and represent a range of projected risks when converted to cancer mortality risks on the basis of FGR 13. The implied excess cancer mortality risks are centered at about 10^{-6} y^{-1} and for most radionuclides, fall in the range 10^{-7} y^{-1} - 10^{-5} y^{-1}, where "y^{-1}" refers to intake over a one-year period. For example, for the 15 primary radionuclides addressed in the present report, these standards correspond to projected excess cancer mortality risks ranging from $3x10^{-7}$ y^{-1} to $7x10^{-6}$ y^{-1} with a median value of about 10-6 y^{-1}. Thus, the value 10^{-6} y^{-1} appears to be a representative value for excess cancer mortality risks implied by current EPA standards for water and air. This value was used as the reference risk for the purpose of deriving Risk-Based Criteria for radionuclides. That is, the risk-based criterion for a radionuclide in water or air is the activity concentration, or the equivalent mass concentration, projected to result in an excess cancer mortality risk of 10^{-6} due to intake over a one-year period.

Risk-Based Criteria for water are based on intake of 2 L d^{-1}, a value commonly used by EPA in development of guidance concerning consumption of water (EPA 1996, EPA 2000). Risk-Based Criteria for air are based on intake of 17.8 m^3 d^{-1}, which is the population-averaged air intake rate estimated in FGR 13.

Risk-Based Criteria for uranium-238 were based on the assumption that uranium 238 is accompanied by uranium-234 and uranium-235 in water and air. For any mixture of these three uranium isotopes, the derived risk-based activity criterion for water is in the range 30-33 pCi L^{-1}, and the derived risk-based activity criterion for air is in the range 0.014-0.017 pCi m^{-3}. The weak dependence of the risk-based activity criteria on the isotopic ratio results from the fact that the risk coefficients for uranium-238, uranium-235, and uranium-234, which are given in FGR 13 as risk per unit activity taken into the body, differ little from one another for a given mode of intake. On the other hand, the risk-based mass criterion of uranium-238 in water or air depends strongly on the relative activities of these three uranium isotopes because the three isotopes have considerably different specific activities. The specific activity of uranium-234 is almost 20,000 times that of uranium-238 and almost 3000 times that of uranium-235. The risk-based mass criterion is a particularly important consideration for uranium because uranium presents a chemical hazard (nephrotoxicity) as well as a radiological hazard, and the chemical hazard generally is measured in terms of the mass of uranium taken into the body or the mass that accumulates in the kidneys.

The specific activity of a mixture of uranium-238, uranium-235, and uranium-234 is at least 0.34 pCi μg^{-1} (the specific activity of uranium-238) and may be higher by an order of magnitude or more for uranium enriched in uranium-235. The specific activity of natural uranium, which is approximately 99.27% uranium-238, 0.72% uranium-235, and 0.0057% uranium-234 by mass, is 0.67 pCi μg^{-1}. The specific activity of uranium in drinking water generally is higher than that of natural uranium due to an elevated concentration of uranium-234 in drinking water relative to natural uranium (Karpas et al. 2005). Typical values for the specific activity of uranium in drinking water in the range 0.8-1.3 pCi μg^{-1} have been estimated from isotopic compositions of uranium found in public water systems (Federal Register 56, July 18, 1991; Wong et al. 1999; EPA 2007b). In the present report, a rounded central estimate of 1 pCi μg^{-1} is used as the specific activity of uranium in drinking water and for consistency is also applied to air. Risk coefficients for uranium-234, which are slightly higher than those for uranium 238 and uranium-235, are applied in the derivations of risk-based activity criteria for uranium-238 in water or air. The resulting risk-based activity criterion and risk-based mass criterion for uranium-238 in water are 30 pCi L^{-1} and 30 μg L^{-1}, respectively. These values are consistent with the current EPA standard for uranium in drinking water, as summarized in the following EPA Memorandum (EPA 2007b):

> "The 2000 MCL [Maximum Contaminant Level] rule established an MCL for uranium of 30 micrograms per liter (μg/L). For the MCL rulemaking, EPA assumed a typical conversion factor of 0.9 pCi/μg for the mix of uranium isotopes found at public water systems, which means that an MCL of 30 μg/L will typically correspond to 27 pCi/L. EPA considered the 30 μg/L level (which corresponds to a 27 pCi/L level) to be appropriate since it is protective for both kidney toxicity and cancer. However, the relationship between mass concentration (μg/L) and activity (pCi/L) is dependent upon the relative mix of the radioactive isotopes (e.g., uranium-234, uranium-235, uranium-238) that comprise the uranium at

> a particular drinking water source. In circumstances with more extreme conversion factors (> 1.5 pCi/µg), uranium activity levels may exceed 40 pCi/L. In these circumstances, EPA recommends in the 2000 MCL rule that drinking water systems mitigate uranium levels to 30 pCi/L or less, to provide greater assurance that adequate protection from cancer health effects is being afforded…"

The derived risk-based activity criterion for uranium-238 in air, 0.014 pCi m^{-3}, was based on the risk coefficient for inhalation of a moderately soluble form of uranium-234 (Type M) because this is the default absorption type identified in FGR 13 for uranium isotopes. The corresponding risk-based mass criterion is 0.014 µg m^{-3}. Based on the biokinetic model for uranium applied in FGR 13, the projected kidney concentration from long-term exposure to this concentration of uranium in air would remain below 0.001 µg g^{-1}, regardless of the inhaled form of uranium. Renal effects of uranium have not been observed below estimated kidney concentrations of a few tenths of a microgram per gram.

As explained below, the Risk-Based Criteria for the primary radionuclides other than uranium-238 were derived under the assumption that there is no intake of accompanying radioactive progeny. However, each of the risk coefficients used to derive the risk-based criteria in Table 11 reflects the contribution of potentially significant radioactive progeny (those listed in Table 10) produced in the body after intake of the parent radionuclide. The contributions of the radioactive progeny to these risk coefficients are particularly important for four of the primary radionuclides: cesium-137, ruthenium-106, radium-226, and strontium-90.

Four of the 15 primary radionuclides, cobalt-60, europium-154, iridium-192, and polonium-210, have no radioactive progeny. No radioactive progeny are listed in Table 10 for five other primary radionuclides, americium-241, californium-252, curium-244, plutonium-238, and plutonium-239, because the progeny grow in only slowly and would present little risk compared with the parent over the first century after release of the parent into the environment.

Relative activities of members of the radium-226 chain in water or air are difficult to predict due to the high mobility of the first daughter in the decay chain, the inert gas radon-222. The derived Risk-Based Criteria for radium-226 listed in Table 11 would change little if it were assumed that radium-226 is in equilibrium with its relatively short-lived daughters, meaning the decay chain members down to, but not including, lead-210. The presence of significant activities of lead-210 and subsequent members of the chain relative to the activity of radium-226 over an extended exposure period seems unlikely. Lead-210 would grow in only slowly and would not be expected to remain with the higher chain members in air or water for an extended period even if the radium-226 decay chain were in equilibrium when the original release occurred.

Each of the primary radionuclides cesium-137, ruthenium-103, ruthenium-106, and strontium-90 gives rise to a short-lived daughter that quickly comes into equilibrium with the parent and is expected to have an activity concentration similar to that of the parent radionuclide in water or air. For each of these four primary radionuclides, however, intake of the daughter in water or air can be neglected because the projected tissue doses and cancer risk are negligible compared with the projected doses and risk from intake of the parent. This is illustrated by intake of ruthenium-106 and its daughter rhodium-106 in drinking water. As indicated in Table 10, the radiological half-life of ruthenium-106 is about 1 year, the radiological half-life of rhodium-106 is about 30 seconds, and decay of a rhodium-106 atom results in considerably greater release of energy than decay of a ruthenium-106 atom. Decay of a ruthenium-106 atom gives rise to an atom of rhodium-106, which soon decays due to the short half-life of rhodium-106. This means that these two radionuclides quickly come into equilibrium, that is, their activities (decays per unit time) are expected to be about the same in drinking water, although the number of ruthenium-106 atoms would remain about six orders of magnitude higher than the number of rhodium-106 atoms due to the difference in half-lives. Intake of drinking water would result in intake of about one million atoms of ruthenium-106 for each atom of rhodium-106 taken into the body, so that the dose and risk from intake of rhodium-106 would be trivial compared with that from intake of ruthenium-106 despite the much higher energy per decay represented by rhodium-106.

Some of the radioactive progeny that represent little additional dose or risk due to their intake in water or air may represent important or even dominant sources of dose and risk after intake of the parent due to production and decay of the progeny in the human body. As an illustration, again consider the parent-daughter pair ruthenium-106 and its daughter rhodium-106. Each decay of ruthenium-106 in the body gives rise to a rhodium-106 atom that quickly decays and deposits considerably more energy in body tissues than was deposited by the preceding decay of ruthenium-106. Due to the much higher energy associated with rhodium-106 decay than with ruthenium-106 decay, rhodium-106 produced in the body is estimated to represent more than 99% of the dose and risk resulting from intake of ruthenium-106. Thus, although intake of rhodium-106 accompanying ruthenium-106 in drinking water or air is unimportant compared with intake of ruthenium-106, the production and decay of rhodium-106 in the body is by far the dominant source of risk from ingested or inhaled ruthenium-106.

Table 10 **Nuclear Decay Data[a] for Primary Radionuclides and Potentially Important Radioactive Progeny**

				Energy (MeV per nuclear transformation)					
				Prominent alpha			Prominent photon		
Radionuclide[c]	**Half-life**	**Decay mode[b]**	**Total alpha**	**Yield (%)**	**Energy**	**Total photon**	**Yield (%)**	**Energy**	**Total electron[d]**
Americium-241	432 y	α	5.48	84.7	5.49	0.029	35.9	0.06	0.037
Californium-252	2.65 y	α SF	5.92	81.5	6.12	<0.01	2.32	0.02	0.006
Cesium-137	30.2 y	β-	-	-	-	<0.01	<0.01	0.283	0.188
Barium-137m	*2.55 m*	*IT*	-	-	-	*0.596*	*89.74*	*0.662*	*0.065*
Cobalt-60	5.27 y	β-	-	-	-	2.504	99.98	1.332	0.097
Curium-244	18.1 y	α SF	5.79	76.4	5.8	<0.01	3.19	0.018	0.008
Europium-154	8.59 y	β- EC	-	-	-	1.249	40.56	0.123	0.273
Iridium-192	73.8 d	β- EC	-	-	-	0.816	82.71	0.317	0.218
Plutonium-238	87.7 y	α SF	5.49	70.9	5.5	<0.01	3.94	0.017	0.011
Plutonium-239	24,000 y	α	5.15	70.7	5.16	<0.01	1.6	0.014	0.007
Polonium-210	138.4 d	α	5.3	100	5.3	<0.01	<0.01	0.803	<0.001

				Energy (MeV per nuclear transformation)					
				Prominent alpha			**Prominent photon**		
Radionuclide[c]	**Half-life**	**Decay mode[b]**	**Total alpha**	**Yield (%)**	**Energy**	**Total photon**	**Yield (%)**	**Energy**	**Total electron[d]**
Radium-226	1600 y	α	4.77	94.4	4.78	<0.01	3.59	0.186	0.004
Radon-222	*3.82 d*	α	*5.49*	*99.9*	*5.49*	*<0.01*	*0.08*	*0.51*	*<0.001*
Polonium-218	*3.10 m*	*α β-*	*6*	*100*	*6*	-	-	-	*<0.001*
Lead-214	*26.8 m*	*β-*	-	-	-	*0.253*	*37.6*	*0.352*	*0.295*
Astatine-218	*1.5 s*	*α β-*	*6.68*	*89.9*	*6.69*	-	-	-	*0.001*
Bismuth-214	*19.9 m*	*β- α*	*<0.1*	*0*	*5.45*	*1.479*	*46.1*	*0.609*	*0.663*
Polonium-214	*0.00016 s*	α	*7.69*	*100*	*7.69*	*<0.01*	*0.01*	*0.8*	*<0.001*
Thallium-210	*1.3 m*	*β-*	-	-	-	*2.763*	*98.96*	*0.8*	*1.27*
Lead-210	*22.2 y*	*β- α*	*<0.1*	*<0.01*	*3.72*	*<0.01*	*10.11*	*0.011*	*0.04*
Bismuth-210	*5.0 d*	*β- α*	*<0.1*	*<0.01*	*4.64*	*<0.01*	*<0.01*	*0.304*	*0.389*
Polonium-210	*138.4 d*	α	*5.3*	*100*	*5.3*	*<0.01*	*<0.01*	*0.803*	*<0.001*
Mercury-206	*8.15 m*	*β-*	-	-	-	*0.122*	*31*	*0.305*	*0.421*
Thallium-206	*4.2 m*	*β-*	-	-	-	*<0.01*	*0.04*	*0.075*	*0.54*
Ruthenium-103	39.3 d	β-	-	-	-	0.496	91	0.497	0.066
Rhodium-103m	*56.1 m*	*IT*	-	-	-	*<0.01*	*4.02*	*0.02*	*0.038*
Ruthenium-106	373.6 d	β-	-	-	-	-	-	-	0.01
Rhodium-106	*29.8 s*	*β-*	-	-	-	*0.206*	*20.4*	*0.512*	*1.411*
Strontium-90	28.8 y	β-	-	-	-	-	-	-	0.196
Yttrium-90	*64.1 h*	*β-*	-	-	-	*<0.01*	*<0.01*	*0.016*	*0.933*
Uranium-238	4.5×10^9 y	α SF	4.19	79	4.2	<0.01	3.04	0.016	0.009
Thorium-234	*24.1 d*	*β-*	-	-	-	*0.011*	*4.84*	*0.063*	*0.062*
Protactinium-234m	*1.17 m*	*β- IT*	-	-	-	*0.016*	*0.84*	*1.001*	*0.817*
Protactinium-234	*6.70 h*	*β-*	-	-	-	*1.472*	*33.41*	*0.014*	*0.404*
Uranium-234	*250,000 y*	α	*4.76*	*71.4*	*4.78*	*<0.01*	*4.18*	*0.016*	*0.014*
Thorium-230	*75,000 y*	α	*4.67*	*76.4*	*4.69*	*<0.01*	*3.32*	*0.015*	*0.015*
Radium-226[e]	*1600 y*	α	*4.77*	*94.4*	*4.78*	*<0.01*	*3.59*	*0.186*	*0.004*

y = year, d = day, m = minute, s = seconds, MeV = million electron volts

[a] Data from compilation by Endo et al. (2005).

[b] α= alpha emission, β- = beta-negative emission, SF = spontaneous fission (nuclear fission occurring without the striking of the atom by a neutron or other particle), IT = isomeric transition (process in which energy is released by emission of a photon, resulting in an atom with the same mass number and atomic number but with a more stable configuration), EC = electron capture (process in which an electron in an atom's inner shell is drawn into the nucleus and combines with a proton, forming a neutron and a neutrino; the neutrino is ejected from the atom's nucleus).

[c] Italicized radionuclides following a primary radionuclide are its decay chain members (radioactive progeny). Cobalt-60, europium-154, iridium-192, and polonium-210 have no radioactive progeny. Radioactive progeny of americium-241, californium 252, curium-244, plutonium-238, and plutonium-239 are not listed because their activity is insignificant compared with that of the parent for decades after entry of the parent into the environment or the human body.

[d] Continuous electron spectrum (beta spectrum) plus discrete mono-energetic electrons.

[e] Uranium-238 chain continues with radium-226 progeny shown earlier in table.

Table 11 Risk-Based Criteria for Primary Radionuclides in Water and Air

Radionuclide	Specific Activity *(Ci/g)*	Water[a]		Air[b]	
		(pCi/L)	*(μg/L)*	*(pCi/m³)*	*(μg/m³)*
Americium-241	3.4	18	5.3×10^{-6}	0.0063	1.9×10^{-9}
Californium-252[c,d]	540	16	3.0×10^{-8}	0.0036	6.7×10^{-12}
Cesium-137	86	65	7.6×10^{-7}	19	2.2×10^{-7}
Cobalt-60	1,100	130	1.2×10^{-7}	5.2	4.7×10^{-9}
Curium-244	81	23	2.8×10^{-7}	0.0068	8.4×10^{-11}
Europium-154[d]	270	230	8.5×10^{-7}	0.89	3.3×10^{-9}
Iridium-192[d]	9,200	330	3.6×10^{-8}	7.2	7.8×10^{-10}
Plutonium-238	17	13	7.6×10^{-7}	0.0052	3.1×10^{-10}
Plutonium-239	0.062	13	2.1×10^{-4}	0.0052	8.4×10^{-8}
Polonium-210	4,500	5.0	1.1×10^{-9}	0.015	3.3×10^{-12}
Radium-226	1.0	5.2	5.2×10^{-6}	0.014	1.4×10^{-8}
Ruthenium-103	32,000	630	2.0×10^{-8}	20	6.3×10^{-10}
Ruthenium-106	3,300	57	1.7×10^{-8}	1.7	5.2×10^{-10}
Strontium-90	140	28	2.0×10^{-7}	1.6	1.1×10^{-8}
Uranium-238[e]	10^{-6}	30	30	0.014	1.4×10^{-2}

[a] Based on a reference risk of 10^{-6} y^{-1} and water intake of 2 L d^{-1}.

[b] Based on a reference risk of 10^{-6} y^{-1} and air intake of 17.8 m^3 d^{-1}.

[c] Californium-252 is not addressed in FGR 13 (EPA 1999). Risk coefficients for californium-252 for use in the present report were derived using the methods of FGR 13 and the current biokinetic and dosimetric models of the ICRP as summarized in ICRP Publication 72 (ICRP 1996). The derived risk coefficients for ingestion and inhalation are 2.30×10^{-9} Bq^{-1} (8.52×10^{-11} pCi^{-1}) and 1.15×10^{-6} Bq^{-1} (4.26×10^{-8} pCi^{-1}), respectively.

[d] No default absorption type for this radionuclide is identified in FGR 13 (EPA 1999) or ICRP Publication 72 (1996). The risk-based criterion for air is based on the maximum of the risk coefficients for inhalation of Type F, Type M, and Type S material.

[e] The specific activity of uranium-238 is 3.4×10^{-7} Ci/g. It was assumed in the derivation of risk-based chronic exposure criteria for uranium-238 in water and air that uranium-238 is accompanied by uranium-235 and uranium-234. The specific activity of the mixture of the three uranium isotopes is assumed to be 10^{-6} Ci/g (1 pCi/μg). The risk-based chronic exposure criteria listed for uranium-238 are intended for application to any mixture of uranium-238, uranium-235, and uranium-234.

5 Summary and Discussion

Water and air were reviewed for more than approximately 100 contaminants identified in the NHSRC list and SAM report combined. Chronic public benchmarks were emphasized, to support validation of analytical methods. These evaluations were phased, beginning with the set of 23 chemicals identified as validation priorities. Companion fate analyses were conducted to identify associated products expected to form in air and water over different intervals. Benchmarks were then further reviewed for those products.

After completing the evaluation for the initial priority set, this benchmark assessment was extended to the entire NHSRC list and SAM report to pursue full coverage for method validation. In concert, physical-chemical fates were analyzed for all the industrial chemicals and agents, and physical fate was assessed for the radionuclides. Benchmarks were then reviewed for these further sets and also for the biological contaminants. Following thousands of checks to assess hundreds of contaminants and fate products combined across a dozen benchmarks, more than 200 distinct risk-based criteria were identified as validation targets. These concentrations are summarized in Table 12. The majority are from EPA benchmarks, with most based on environmental exposures that are assumed to continue for decades. Where multiple relevant benchmarks exist, EPA values are prioritized; the emphasis is on values that reflect most recent evaluations.

5.1 Fate Products

Fate analyses provide essential input to method validation; some of these associated chemicals can accompany the primary contaminants when released (e.g., chemical agents), depending on the synthesis and release methods. This fate overview emphasizes key products. It is noted that the yields, stability and toxicity of numerous agent fate compounds indicate that many are of little to no significant health concern, especially when compared to characteristics of the parent compound (Talmage et al 2007).

Table 12 Summary of Risk-Based Criteria as Analytical Method Validation Targets for Water and Air[a]

Contaminant	CAS RN	Concn. in Water *($\mu g/L$)*	Concn. in Air *($\mu g/m^3$)*
Chemicals			
Acetone	67-64-1	32,000	
Aldicarb (Temik)	116-06-3	35	
Aldicarb sulfone	1646-88-4	35	
Aldicarb sulfoxide	1646-87-3	35	
Allyl alcohol	107-18-6	180	
Ammonia, anhydrous ammonia	7664-41-7	34,000	100 *(70)*
Arsenic, inorganic (including trivalent)	7440-38-2	10	0.0002
Arsine (agent SA, arsenic hydride)	7784-42-1		0.05
Asbestos (can exist in various forms)	1332-21-4	(210) 7 M f/L	(0.012) 400 f/m^3
Benzene (gasoline range organics)	71-43-2	5	0.13
Boric acid (as B equivalents in water)	10043-35-3	10,500	
Boron trichloride *(as B^- in water)*	10294-34-5	(7,000)	
Boron trifluoride *(as F^- in water)*	7637-07-2	(2,100) *(1,400)*	0.7
Bromadiolone	28772-56-7	(0.7)	
Cadmium	7440-43-9	5	0.0006
Carbofuran	1563-66-2	40	
Carbon disulfide	75-15-0	3,500	700
Carbon monoxide	630-08-0		10,000
Chlorine	7782-50-5	4,000	0.2
2-Chloroethanol (ethylene chlorohydrin)	107-07-3		
Chloropicrin (formerly agent PS)	76-06-2	50	0.4
2-Chlorovinylarsonous acid (CVAA)	85090-33-1	(3.5)	0.11
Cyanide (CN^-), free	57-12-5	200	9
Cyanide salts, as sodium cyanide for water, as CN compounds in air (Cal/EPA, CAS 1-07-3)	143-33-9	1,400	9
Cyanogen chloride (agent CK)	506-77-4	1,800 *(750)*	9.0
Cyclohexyl sarin (agent GF, cyclosarin)	329-99-7	0.14	0.001
Dichloroacetic acid	79-43-6	60	
1,2-Dichloroethane (ethylene dichloride)	107-06-2	5	0.04
Dichlorvos	62-73-7	0.28	0.5
Dicrotophos (Bidrin)	141-66-2	3.5 *(0.2)*	NA
NA Diesel engine exhaust (mixture) CAS, Cal/EPA	(9-91-1)		5 *(0.33)*
2-Diisopropylaminoethanol	96-80-0	290	10
S-[2-(diisopropylamino)ethyl]MPTA (EA 2192)	73207-98-4	0.021	0.0007
Diisopropyl ethyl mercaptoamine (DESH)	5842-07-9	130	4.6
1,2-Diisopropyl methylphosphonate (DIMP)	1445-75-6	2,800 *(600)*	
Dimethyl phosphite (DMP or DMHP)	868-85-9	1,500	420
Dimethylamine	124-40-3		2
1,4-Dithiane (diethylene disulfide)	505-29-3	350 *(80)*	
Divinyl sulfone	77-77-0	(0.25)	
Ethyl sarin (agent GE)	1189-87-3	(0.7)	NA
Ethylbenzene (gasoline range organics)	100-41-4	700	1,000
Ethylene glycol	107-21-1	70,000 *(14,000)*	400
Ethylene oxide (Oxirane)	75-21-8	8	30 *(1.1)*
O-ethyl methylphosphonic acid (EMPA)	1832-53-7	980	34
O-ethyl methylphosphonothioic acid (EMPTA)	18005-40-8	250	8.5
Fenamiphos	22224-92-6	8.8 *(1)*	(1.4)
Fenamiphos sulfone	31972-44-8	(8.8) *(1)*	(1.4)
Fenamiphos sulfoxide	31972-43-7	(8.8) *(1)*	(1.4)
Fluorine *(as soluble F^- in water, HF in air)*	7782-41-4	4,000	(14)
Formaldehyde	50-00-0	7,000 *(1,000)*	0.08
Furan	110-00-9	35	
Gasoline (CAS number is for gasoline vapors)	1-11-0		2,100
n-Hexane (gasoline range organics)	110-54-3	2,100	700
Hydrogen chloride (HCl)	7647-01-0		20 *(9)*
Hydrogen cyanide (HCN, agent AC)	74-90-8	700	3
Hydrogen fluoride (HF) (as F^- in water)	7664-39-3	4,000	14
Hydrogen sulfide	7783-06-4	200	2
Isopropanol	67-63-0		7,000
Isopropyl methylphosphonic acid (IMPA)	1832-54-8	3,500 *(700)*	
Kerosene	8008-20-6		10
Lewisite-1 (agent L-1)	541-25-3	3.5	3

Table 12 **Summary of Risk-Based Criteria as Analytical Method Validation Targets for Water and Air**[a]

Contaminant	CAS RN	Water Concn (*µg/L*)	Air Concn (*µg/m³*)
Lewisite-2 (agent L-2)	40334-69-8	(3.5)	(3)
Lewisite-3 (agent L-3)	40334-70-1	(3.5)	(3)
Lewisite oxide	3088-37-7	(3.5)	0.11
Mercuric chloride, as mercury (inorganic)	7487-94-7	11 *(2)*	0.09
Methanol	67-56-1	18,000	4,000
Methyl isocyanate	624-83-9		1
Methyl paraoxon	950-35-6	(0.88)*(0.2/0.018)*	0.01
Methyl parathion	298-00-0	8.8 *(2/0.18)*	0.01
Methylphosphonic acid (MPA)	993-13-5	700	24
Mevinphos (Phosdrin)	7786-34-7	8.8	
Mustard, sulfur (agent H) and distilled agent HD	505-60-2	0.25	0.02
Mustard HT (agent HT: 60% HD, 40% T)	HD: 505-60-2 T: 63918-89-8	0.25	0.02
Mustard sulfone	471-03-4	(0.25)	(0.02)
Mustard sulfoxide	5819-08-9	(0.25)	(0.02)
Nicotine	54-11-5	70	
Nitrate (NO_3^-)	14797-55-8	10,000	
Nitric acid (fuming, FNA) *(as nitrate in water)*	7697-37-2	(10,000)	(86)
Nitrogen oxides *(as NO_2; nitrite in water)*	10102-44-0	(1,000)	100
p-Nitrophenol (para- or 4-nitrophenol)	100-02-7	280	0.1
Oxamyl (Vydate)	23135-22-0	200	
Ozone (O_3)	10028-15-6		160
Paraquat (dichloride)	1910-42-5	160 *(30)*	(0.01)
Perfluoroisobutylene (PFIB)	382-21-8		(0.3)
Phenol	108-95-2	11,000 *(2,000)*	200
Phorate (Thimet)	298-02-2	7	
Phorate sulfone	2588-04-7	6	
Phorate sulfoxide	2588-03-6	6	
Phosgene	75-44-5		0.3
Phosphine	7803-51-2	11	0.3
Phosphoric acid	7664-38-2	12,000	10
Polychlorinated biphenyls (PCBs)	1336-36-3	0.5	0.01
Propylene oxide	75-56-9	0.1	0.3
Red phosphorous (RP)	7723-14-0	(0.7) *(0.1)*	(10)
Sarin (agent GB)	107-44-8	0.7	0.001
Sodium fluoroacetate (for fluoroacetate salts)	62-74-8	0.7	
Soman (agent GD)	96-64-0	0.14	0.001
Strychnine	57-24-9	11	
Sulfate (for air, Cal/EPA lists as CAS 9-96-0)	9-96-0	500,000	25
Sulfur dioxide *(as sulfate in water, see above)*	7446-09-5	(500,000)	79
Sulfuric acid *(as sulfate in water)*	7664-93-9	(250,000)	1
Tabun (agent GA)	77-81-6	1.4	0.001
Tear gas (agent CS, per form CN, 532-27-4)	2698-41-1		(0.03)
Thiodiglycol (TDG)	111-48-8	14,000	
Titanium tetrachloride (agent FM)	7550-45-0		0.1
Toluene (gasoline range organics)	108-88-3	1,000	5,000 *(300)*
Trimethyl phosphite (TMP)	121-45-9	(1,500)	
VX	50782-69-9	0.021	0.0006
Xylenes (gasoline range organics)	1330-20-7	10,000	100
Radionuclides			
Americium-241 (7440-35-9)	14596-10-2	5.3×10^{-6}	1.9×10^{-9}
Californium-252 (7440-71-3)	13981-17-4	3.0×10^{-8}	6.7×10^{-12}
Cesium-137 (7440-46-2)	10045-97-3	7.6×10^{-7}	2.2×10^{-7}
Cobalt-60 (7440-48-4)	10198-40-0	1.2×10^{-7}	4.7×10^{-9}
Curium-244 (7440-51-9)	13981-15-2	2.8×10^{-7}	8.4×10^{-11}
Europium-154	15585-10-1	8.5×10^{-7}	3.3×10^{-9}
Iridium-192	14694-69-0	3.6×10^{-8}	7.8×10^{-10}
Plutonium-238 (7440-07-5)	13981-16-3	7.6×10^{-7}	3.1×10^{-10}
Plutonium-239 (7440-07-5)	15177-48-3	2.1×10^{-4}	8.4×10^{-8}
Polonium-210 (7440-08-6)	13981-52-7	1.1×10^{-9}	3.3×10^{-12}
Radium-226 (7440-14-4)	13982-63-3	5.2×10^{-6}	1.4×10^{-8}
Ruthenium-103	13968-53-1	2.0×10^{-8}	6.3×10^{-10}
Ruthenium-106	13967-48-1	1.7×10^{-8}	5.2×10^{-10}
Strontium-90 (7440-24-6)	10098-97-2	2.0×10^{-7}	1.1×10^{-8}
Uranium-238 *(7440-61-1)*	7440-61-1	30	1.4×10^{-2}

[a] This table summarizes risk-based criteria (direct and indirect) for potential contaminants in water or air, covering distinct threat contaminants (over 60 chemicals and 15 radionuclides) and multiple chemical fate products. Fate products of chemicals from the NHSRC list are italicized; some are also main contaminants in the SAM report (e.g., CVAA, EMPA, IMPA, and MPA). All 15 radionuclides have values for water (100%). For the radionuclides, the CAS RNs in parentheses are for the element. The elemental and isotopic CAS RNs for uranium-238 are the same, as essentially all natural uranium is uranium-238 (by mass). Air values are identified for all 15 radionuclides (100%). Values are provided for both air and water for more than 50% of the contaminants including all 15 radionuclides. These include indicators derived from data for pesticides (for air, a few are based on applicator assessments but are included here to provide initial bounding context for method validation). Note the nitrite CAS is 14797-65-0.

Nitric acid, fuming, is on the NHSRC list; its CAS number is the same as for nitric acid (concentrated to >86%); the air benchmark is for nitric acid not distinguished as fuming. Sulfuric acid (from the NHSRC list) is hydrogen sulfate, represented in water by sulfate. The category "gasoline range organics" from the SAM report is represented by 5 chemicals: BTEX and n-hexane. For the radionuclides, other CAS numbers identified for these elements are given in parentheses. To facilitate comparisons, all values are provided as μg /L for water and μg/m^3 for air. For asbestos, the conversion of 30 μg/m^3 per f/mL (in IRIS) was used to support these direct comparisons, but values corresponding to the actual benchmarks as fibers are also shown (see Table 9 and footnote). Shading indicates that directly relevant public benchmarks were not found, and parentheses indicate that the concentration was derived or is represented by a related compound. The value for n-hexane in water is the 10-d HA for a 10-kg child (no chronic limit was identified). Values for 2-chloroethanol, ethylene oxide, and nicotine are initial indicators scaled from food residue tolerances to offer preliminary context for validation. When a lower non-EPA benchmark exists, it is shown in italics and parentheses, with lighter font (green). The values from most recent studies are prioritized. Also, final values are prioritized over those identified as draft or under review. These other values are included to offer further context for validation. From the initial review of readily available data, no chronic public benchmarks were found for 21 chemicals shown in Box 4. The 10 for which no chronic occupational limits were identified in the initial review are in bold. For example, although no environmental benchmarks exist for the drugs heroin and PCP, a relevant therapeutic benchmark exists for heroin, and medical data exist for PCP. Preliminary internal data analyses suggest a possible upper bound for heroin in drinking water on the order of the IMPA concentration (3,500 μg/L), while a possible bound for PCP might be 10 times lower, on the order of that for 1,4-dithiane.

Chemicals in NHSRC List or SAM Report Without Chronic Public Benchmarks (Box 4)

(not found in this review; those also without standard occupational limits are in bold)

NHSRC List		SAM Report	
Chemical	***General Type***	***Chemical***	***General Type***
Crimidine	pesticide	**3-Chloro-1,2-propanediol** *(alphachlorohydrin)*	pesticide
Diacetylmorphine (heroin)	drug	**Chlorosarin**	chemical agent precursor
Diborane	toxic industrial chemical (TIC)	**Chlorosoman**	chemical agent precursor
Ethyldichloroarsine	chemical agent	**Dimethylphosphoramidic acid**	agent (tabun) hydrolysis product
Hydrogen bromide	TIC; pesticide fate product	Methyl hydrazine	TIC, used in pesticide synthesis
Methoxyethylmercuric acetate	pesticide	Methylamine	TIC, used to make methamphetamine, microcystin biotoxin component
Methyl fluoroacetate	pesticide	Osmium tetroxide	TIC, used in microscopy stains, possible agent
Nitrogen mustard	chemical agent	**1,4-Thioxane**	agent (sulfur mustard) fate product and impurity
Phencyclidine *(angel dust, PCP)*	drug		
Phosphorus trichloride	TIC; pesticide and agent precursor		
Tetraethyl pyrophosphate	pesticide		
Tetramethylene disulfotetramine	pesticide (rat poison)		
Tungsten hexafluoride	TIC (for bullets, semiconductors)		

Fate products of priority chemical contaminants and additional chemical agents with health-based benchmarks are italicized in the individual results Tables 5 to 8 (Chapter 4). For the radionuclides, radioactive progeny of potential dosimetric importance are listed in Table 10. With the exception of certain members of the uranium-238 decay chain, it was concluded that intake of accompanying radioactive progeny in water or air typically would not add significantly to the radiation dose resulting from intake of the primary radionuclide.

Of the primary contaminants and fate products assessed, many are volatile or SVOCs. These can be lost from air via three primary mechanisms: (1) reaction with the hydroxyl radical or other reactive species such as ozone and nitrate radicals; (2) wet deposition, or washout; and (3) dry deposition, or gravitational settling. The atmospheric lifetime of volatile organic compounds (VOCs) is generally determined by their chemical reactivity with the hydroxyl radical in the atmosphere. Highly reactive compounds such as alkenes, or olefins (e.g., allyl alcohol), react rapidly with this radical, so atmospheric lifetimes are on the order of hours to a day. The reaction rates for more stable alkane compounds such as ethane and propane are a function of the length of the carbon chain. For example, decane (with ten carbons, which typically constitutes 20% of kerosene, a contaminant from the SAM report) would react with a lifetime of less than a day, while ethane (with two carbons) would react much more slowly, with a lifetime on the order of a month. Thus, VOCs exhibit a range of atmospheric lifetimes that can extend from hours to months.

SVOCs will also react with hydroxyl radicals in the atmosphere but at a much slower rate. Primary loss for these compounds is due to their partitioning from the gas to the particle phase in the atmosphere. The tendency to partition into the gas phase is a function of temperature, with more of the compound in the particle phase at colder temperatures. Once in that phase, contaminants would be removed from the atmosphere at the same rate as the particle washout rate, which generally ranges from a week to a month depending on geographical location. However, certain semivolatile compounds can persist in the atmosphere for a long time, in some cases for more than a year; this has led that group of chemicals to be referred to as persistent organic pollutants. Their atmospheric persistence is thought to result from the distillation effect, which reflects the tendency of gases to re-evaporate in warmer seasons after being deposited onto surfaces, then repartition into the particle phase during the next cold spell. This process has generally resulted in these pollutants migrating north toward cold polar regions.

This discussion is relevant to the portion of a given compound such as a pesticide that is in the vapor phase and hence transportable in air. As a practical matter, if SVOCs were sprayed (e.g., from an airplane or mechanical sprayer), not all of the chemical would be expected to exist in the gas phase. Under those conditions, small droplets or aerosols would likely exist, which would stick to earth or plant surfaces relatively quickly due to gravitational settling. Thus, this aerosolization mechanism (with some portion of a sprayed pesticide naturally vaporized during application) could enhance the adherence of pesticides to such surfaces. Note that atmospheric lifetime here represents how long a species typically resides in the atmosphere before being removed; it is mathematically defined as the time it takes the initial concentration of the given species to decrease by a factor of $1/e$ (or 1/2.72), e.g., following a discrete release. For example, if 100 g/m^3 of a chemical were released to air all at once, then its atmospheric lifetime would be the time it takes that amount to be reduced to 37 g/m^3.

A more extensive fate overview was developed to reflect characteristics of the chemical in that medium, not the basic properties of a pure liquid as reported in common data sources. When quantitative data were not readily available, descriptors of low, medium, or high were estimated from chemical structures using the general categories in Box 5.

Solubility and Volatility Indicators for Chemicals in Water (Box 5)

Property	*Low*	*Medium*	*High*
Solubility	<1,000 ppm	1,000 to 10,000 ppm	≥10,000 ppm
Volatility	>1,000 mol/L atmosphere (atm)	1 to 1,000 mol/L atm	<1 mol/L atm

The volatility descriptor was determined by considering the general magnitude of Henry's Law constant (K_H) for each chemical. This constant describes the equilibrium concentrations in water and overlying air in a closed system. It is useful for evaluating both water solubility and volatility in air, i.e., the vapor pressure or expected vapor pressure of the pure substance. For example, the volatility of chlorine gas (Cl_2) from drinking water would be categorized as high because of its limited water solubility and high vapor pressure, as would the volatility of other similar chemicals that are gases or vapors at typical drinking water temperatures. To estimate the solubility descriptor, the ionization state of the chemical at neutral pH was considered together with the chemical structure. Substances that are ionic at neutral pH were categorized as having high solubility. For example, phosphoric acid, a degradation product of a number of study chemicals, falls in this category because at neutral pH it would primarily exist as the dissociated anion (or in this case, anions). For nonionic chemicals, the presence of particular functional groups was considered in determining the solubility indicator. Solubility was considered high for chemicals with phenolic (OH), carboxylic acid (COOH), or amino (NH_2) groups due to their ability to participate in hydrogen bonding with water. The presence of carbonyl (C=O), ether (C-O-C), or heterocyclic O or N groups was associated with medium solubility. The absence of any of these or other polar groups was associated with low water solubility. Molecular weight was considered a modifying factor, with solubility generally decreasing with increasing molecular weight.

These physical-chemical properties are used to assess whether a chemical in water could be an inhalation threat. With the K_H indicating the ratio of a chemical's volatility to its solubility, it can be used to evaluate the significance of volatilization from water in the following way. Chemicals with a K_H less than 1×10^{-5} atm-m^3/mole and a molecular weight (MW) above 200 g/mole are unlikely to pose an inhalation hazard as a result of volatilization from drinking water in a residential setting (EPA 2004d). To illustrate, consider methyl parathion with a MW of 263 g/mole and a K_H of 1×10^{-7} atm-m^3/mole. If this chemical were released to a drinking water supply, it would not be expected to pose an inhalation hazard. The compound would stay in solution with very little partitioning to air.

This study focuses on low validation targets to support final decontamination. Nevertheless, fate information is also used to indicate what contaminants could best guide the assessment of performance for health protection across response phases, beginning with the release and extending through interim measures to final decontamination. A sentinel or companion "check-contaminant" can also be useful, especially when it can be detected relatively easily and inexpensively. In addition to those readily measured, validation efforts can focus on a core set of contaminants by considering the relative amounts formed. Data on structures and illustrative equations that include molar ratios can be used to indicate those amounts.

Combining fate information with other context, including threat and relative toxicity, can help prioritize validation efforts on those contaminants that matter most for health protection. This approach is straightforward when detection capabilities relative to the target concentrations are similar across persistent chemicals, so assuring baseline validation below health-based levels for those contaminants is key. Fate information also helps identify supporting candidates such as generally benign chemicals that would not pose a health threat to those conducting the analyses.

Certain fate products are associated with a number of threat contaminants, and for these, fate/persistence data can be combined with toxicity data to focus on key surrogates and indicators.

For example, multiple threat chemicals introduced to water would produce hydrogen chloride (HCl) with a relatively short half-life of hours to days. Thus, HCl would be a useful detection indicator as well as a practical surrogate because it would lower the pH of the water, which could be readily detected via in-stream monitoring. Two other highly stable chemicals are fate products for several contaminants: methylphosphonic acid (MPA) and phosphoric acid. These two would also be candidates for broad detection strategies designed to monitor water for potential releases.

In summary, fate information is crucial to effective method validation, in order to understand the type and timing of other contaminants expected to form in water and air after an original chemical is released. It is particularly important for short-lived contaminants, to assure the identification of associated products that could drive health concerns and cleanup issues. The initial fate overview in this report can also be used to frame streamlining and prioritization activities for method validation. Joint consideration of relative toxicity (discussed next) is important for those analyses.

5.2 Benchmark and Method Coverage

With the aim of providing some context for method validation for all chemicals and radionuclides, this report provides risk-based criteria from benchmarks for numerous threat contaminants and fate products. These concentrations cover the majority of the contaminants from the NHSRC list.

This report focuses on chronic benchmarks, so a number of coverage "gaps" are actually appropriate. In contrast, coverage is complete across all radionuclides that would persist with half-lives of more than a month (ruthenium-103) to several billion years (uranium-238). Values are identified for each isotope in both media, with most calculated from standard EPA dose limits.

Gaps are primarily due to incomplete coverage of chemical agents (water and air) and pesticides (air). The same pattern is seen across agents and industrial chemicals in the other contaminant sets.

Of the main threat contaminants with at least one risk-based criteria, most have values for drinking water, and many have values for air. The bulk of the total values identified for the primary contaminants are from directly relevant benchmarks.

For the rest, some are represented by analogues and others are represented by fate products, notably for chemicals that do not persist, such as arsine, nitrogen mustard, and tear gas in water; a few are derived from route-related limits, such as oral tolerances for pesticide residues for bromadiolone, ethylene oxide, and nicotine.

The basic principle of this effort is that when a chronic public benchmark was not found, further sources were evaluated in an effort to provide at least preliminary context for validation targets for all the threat contaminants identified in the NHSRC list and SAM report. This approach provides a basic guide for future research and development.

Part of the further evaluation for chemicals without chronic public benchmarks involved checking occupational levels from OSHA, NIOSH, and ACGIH for workplace air. These limits address exposures of 8 or 10 hours a day and 5 days a week over a working lifetime, which aligns with the chronic duration of interest for this study. Military exposure guidelines for air and water and additional airborne exposure limits for deployed personnel are the primary sources for chemical agents. In contrast to the split for chronic public benchmarks, most (above 80%) are for air. Many address common environmental contaminants for which EPA limits also exist.

This report focuses on chronic public benchmarks. Reviewing occupational benchmarks can support insights regarding other analyses that have been conducted, with an emphasis on limits that are explicitly health-based, such as the TLVs and many (not all) RELs and PELs, and also extending to the German limit, maximale arbeitsplatzkonzentration (MAK). Furthermore, analogues or other surrogates can be considered for insights into relative toxicity.

That information can be combined with emergency response levels for acute exposures such as AEGLs and temporary emergency exposure limits (TEELs) to determine whether integrated comparisons may support bounding context for method validation. Through these further reviews, preliminary information is available as initial support for method validation for at least one medium for all the threat chemicals.

In summary, combining the validation targets developed in this report with the analytical limits from the SAM report highlights opportunities for filling key gaps in both method and benchmark coverage. Follow-on evaluations would be expected to consider three areas: (1) sufficiency of method coverage, for example considering screening and definitive methods and both primary and backup options; (2) more detail regarding analytical limits for individual contaminants, rather than broad ranges, to assure that health-based targets can be adequately measured; and (3) refinement of certain benchmark bases, including to address conservatism (some risk-based criteria are represented by benchmarks for related chemicals, including more toxic parent compounds).

6 Findings

This integrated evaluation of chronic public benchmarks and contaminant fate has identified more than 200 risk-based criteria as method validation targets across numerous contaminants and fate products in drinking water and air combined. The gap in directly applicable values is considerable across the full set of threat contaminants, so preliminary indicators were developed from other well-documented benchmarks to serve as a starting point for validation efforts. By this approach, at least preliminary context is available for water or air, and sometimes both, for all chemicals on the NHSRC list that was provided for this evaluation. This means that a number of concentrations presented in this report represent indirect measures derived from related benchmarks or surrogate chemicals, as described within the results tables.

The main findings of this evaluation to identify risk-based method validation targets are as follows:

1. Chronic benchmarks provide a useful basis for some low risk-based targets for analytical methods. Directly applicable, contaminant-specific public benchmarks for drinking water and air are somewhat limited across the entire suite of contaminants. Coverage is complete for the 15 radionuclides and about half the chemicals.
2. This report provides benchmarks for surrogates or fate products, as well as route-related benchmarks. Food residue limits for several pesticides and safety levels for biological contaminants in foods contribute to further coverage. A risk-based chronic exposure concentration is available in at least one medium for a majority of the threat contaminants. The same split applies as for the direct benchmarks, with more targets available for water than for air.
3. A fate analysis is essential to understanding the identity and timing of relevant degradation products that would form in water and air, so validation targets can also be identified for those compounds posing legitimate concern.
4. For chemicals lacking chronic public benchmarks, workplace limits for long-term exposures can be considered for context, prioritizing those that are explicitly health-based.
5. For chemicals lacking both chronic public and occupational benchmarks, depending on the contaminant and data available, information from acute exposure guidelines (usually derived from a level of health effect) can be compared with other guides and relative toxicity information to develop bounding context for method validation.
6. Preliminary context is provided for method validation in at least one medium for all threat chemicals in the NHSRC list, by integrating information on

related benchmarks, relative toxicity, and fate. One step that can be taken to address benchmark gaps across media is to evaluate the toxicity data for these contaminants, including the data underlying existing benchmarks. Contributions from other routes including dermal exposures also need to be specified where those data exist.

7. A key gap for fate information is the identification of radical oxidation products in air. Although half-lives have been measured or can be generally estimated, specific identities are often missing. This gap limits the determination of benchmarks for a number of specific fate products in air that might pose health concerns.
8. For toxicity gaps, no-observed-adverse-effect levels to support chronic benchmarks are lacking for a number of chemicals, as are quantitative considerations of sensitive subgroups within many existing benchmarks. To fill such gaps, downward adjustments can be applied to account for uncertainty.
9. This report provides information useful in streamlining and prioritizing method validation and health-based evaluations. Fate, relative toxicity, and method limits are considered.

Taken together, this information can be used to guide effective method validation for all the threat contaminants on the NHSRC list.

Other areas that may be considered for further research are as follows:

1. Combine fate, benchmark, and validation data to target the development of quick-turnaround methods for short-lived, relatively toxic contaminants that are considered priority threats per ongoing threat and vulnerability assessments to ensure faster detection (and support faster implementation of exposure controls).
2. Consider whether additional analyses are warranted, particularly for nonpersistent compounds, when detection limits are higher than or close to chronic benchmark concentrations.
3. Address other exposure routes, including dermal absorption, to support route-specific validation targets and route-integrated targets for joint exposures to water and air; include fate/partitioning analyses in addressing multi-route contributions to those combined concentration targets.
4. Assess benchmarks for other durations (subchronic, short-term, and acute) to identify validation targets for initial and intermediate response intervals.
5. Integrate these data to identify broad indicator contaminants for sentinel detection, surrogates, and primary and check contaminants for streamlined validation.
6. Prioritize contaminants with the most significant gaps by overlaying benchmark gaps with fate and toxicity data (and results of ongoing threat and vulnerability assessments); assess other occupational limits (including MAKs), and incorporate context from those and other advisories to refine targets as indicated and determine where few data are available to guide health-based detection (and response).
7. As needed, pursue focused laboratory research to fill gaps in fate product identities (notably from radical oxidation reactions in air) and their persistence,

so analytical methods can be assessed or developed and specific toxicities can be addressed, including via extrapolation approaches.

8. As needed, pursue focused laboratory research and coordinate with ongoing studies to fill gaps in toxicity knowledge; these range from basic toxicity studies to the development of tailored extrapolation methods that incorporate physical, chemical, and toxicological properties through quantitative structure-activity relationships, benchmark dose/concentration analyses, neural networks, and uncertainty analyses with Bayesian belief networks. With this information, analytical methods can be assessed or developed to align with health-based levels.

In summary, health-based information provides a crucial foundation for validation of analytical methods. Gaps identified in this study can help frame research and development for analytical methods as well as related fate and toxicity analyses. Combining information on fate, benchmarks, toxicity, and analytical methods strengthens the validation effort as well as other ongoing health-related research within NHSRC.

7 References

(Includes available Web links and several resources assessed for supporting context.)

Army (U.S. Department of the Army), 2001, Army Chemical Agent Safety Program, Army Regulation 385-61, Headquarters, Washington, DC (12. Oct.); http://www.army.mil/ usapa/epubs/pdf/r385_61.pdf.

ATSDR (Agency for Toxic Substances and Disease Registry), 1992, *Toxicological Profile for Nitrophenols: 2-Nitrophenol, 4-Nitrophenol,* Atlanta, GA (July); http://www.atsdr.cdc. gov/toxprofiles/tp50.pdf.

ATSDR, 1995, *Toxicological Profile for Automotive Gasoline*, Atlanta, GA (June); http://www.atsdr.cdc.gov/toxprofiles/tp72.html.

ATSDR, 1997, *Toxicological Profile for Titanium Tetrachloride*, Atlanta, GA (Sept.); http://www.atsdr.cdc.gov/toxprofiles/tp101.html.

ATSDR, 2001a, *Toxicological Profile for Fluorine, Hydrogen Fluorides, and Fluorides (Draft for Public Comment),* Atlanta, GA (Sept.); http://www.fluorideaction.org/ pesticides/atsdr.fluor.toxprofile.2001.pdf.

ATSDR, 2001b, *Toxicological Profile for Methyl Parathion*, Atlanta, GA (Sept.); http://www.atsdr.cdc.gov/toxprofiles/tp48.html.

ATSDR, 2003a, *Toxicological Profile for Fluorine, Hydrogen Fluorides, and Fluorides (Update),* Atlanta, GA (Sept.); http://www.atsdr.cdc.gov/toxprofiles/tp11.pdf.

ATSDR, 2003b, *Toxicological Profile for Sulfur Mustard (Update)*, Atlanta, GA (Sept.); http://www.atsdr.cdc.gov/toxprofiles/tp49.pdf.

ATSDR, 2005, *ATSDR Minimal Risk Levels (MRLs) for Hazardous Substances*, Atlanta, GA (Dec.); http://www.atsdr.cdc.gov/mrls.html.

ATSDR, 2006, *Medical Management Guidelines for Blister Agents: Nitrogen Mustards*, Atlanta, GA; http://www.atsdr.cdc.gov/MHMI/mmg164.html.

CA Department of Health Services, 2007, Chloropicrin. Available online at http://www.dhs.ca.gov/ps/ddwem/chemicals/AL/PDFs/archive.pdf, archived advisory level.

Cal/EPA (California EPA), 1999, letter from J.R. Froines, Scientific Review Panel, to P.E Helliker, Department of Pesticide Regulation, approving *Evaluation of Methyl Parathion as a Toxic Air Contaminant*, Sacramento, CA (Nov. 3); http://www.arb.ca.gov/srp/srp3.pdf.

Cal/EPA, 2000, *Appendix B, Comparison of Cal/EPA and USEPA Toxicity Values*; within Web site. http://www.oehha.ca.gov/risk/pdf/APENDX-B.pdf.

Cal/EPA, 2003, *Adoption of Chronic Reference Exposure Levels for Fluorides Including Hydrogen Fluoride*, Office of Environmental Health Hazard Assessment, Sacramento, CA (Aug. 15); http://www.oehha.ca.gov/air/chronic_rels/HyFluoCREL.html.

Cal/EPA, 2005a, *Chronic Reference Exposure Levels*, Office of Environmental Health Hazard Assessment, Sacramento, CA (Feb.); http://www.oehha.ca.gov/air/chronic_rels/AllChrels.html.

Cal/EPA, 2005b, *Consolidated Table of OEHHA/ARB Approved Risk Assessment Health Values (Table 1)*, Air Resources Board, Sacramento, CA (April 25); http://www.arb.ca.gov/toxics/ healthval/contable.pdf; within Web site (dated June 2005): http://www.arb.ca.gov/toxics/ healthval/healthval.htm.

Cal/EPA, 2005c, *OEHHA/ARB Chronic Reference Exposure Levels and Target Organs (Table 3)*, Air Resources Board, Sacramento, CA (April 25); http://www.arb.ca.gov/toxics/ healthval/chronic.pdf; within Web site (dated June 2005): http://www.arb.ca.gov/toxics/ healthval/healthval.htm.

Cal/EPA, 2005d, *Air Toxics Hot Spots Program Risk Assessment Guidelines, Part II, Technical Support Document for Describing Available Cancer Potency Factors*, Air Resources Board, Sacramento, CA (May); http://www.oehha.ca.gov/air/hot_spots/pdf/May2005Hotspots.pdf.

Cal/EPA, 2006, *Ambient Air Quality Standards*, Air Resources Board (ARB), Sacramento, CA (May); http://www.arb.ca.gov/aqs/aaqs2.pdf.

CDC (U.S. Department of Health and Human Services, Centers for Disease Control and Prevention), 1988, *Final Recommendations for Protecting the Health and Safety Against Potential Adverse Effects of Long-Term Exposure to Low Doses of Agents GA, GB, VX, Mustard Agent (H, HD, T) and Lewisite (L)*, Federal Register 53(50):8504–8507 (March 15); http://wonder.cdc.gov/wonder/PrevGuid/p0000027/p0000027.asp (Web site last updated 2003).

CDC, 2003, "Final recommendations for protecting human health from potential adverse effects of exposure to agents GA (Tabun), GB (Sarin), and VX." U.S. Department of Health and Human Services, Centers for Disease Control and Prevention. *Federal Register* 68(196): 58348-58351 (October 9).

CDC, 2004, "Interim Recommendations for Airborne Exposure Limits for Chemical Warfare Agents H and HD (Sulfur Mustard)," *Federal Register*, 69 (85): 24164–24168 (May 3); http://www.cdc.gov/nceh/demil/files/Federal%20Register%20Mustard%20AEL%205_2004.pdf.

CDC, 2006, *Bioterrorism Agents/Diseases, Emergency Preparedness and Response*, Atlanta, GA (accessed July 2006); http://www.bt.cdc.gov/agent/agentlist-category.asp.

CHPPM (U.S. Army Center for Health Promotion and Preventive Medicine), 1998 (Web site last updated), *Detailed Facts about Blood Agent Cyanogen Chloride*, Office to the Deputy for Technical Services, Aberdeen Proving Ground, MD; http://chppm-www.apgea.army.mil/dts/docs/detck.pdf.

CHPPM, 1999, *Derivation of Health-Based Environmental Screening levels for Chemical Warfare Agents; A Technical Evaluation*, U. S. Army Center for Health Promotion and Preventive Medicine, Aberdeen Proving Ground, MD.

CHPPM, 2004a, *Chemical Exposure Guidelines for Deployed Military Personnel* (Technical Guide 230, Version 1.3 – Updated May 2003, with January 2004 addendum), Aberdeen Proving Ground, MD; http://chppm-www.apgea.army.mil/documents/TG/TECHGUID/TG230.pdf.

CHPPM, 2004b, *Summary of Chemical Agent Air Exposure Values (Table 1),* noted within OSHA Homeland Security Emergency Preparedness and Response, *Blister Agents* and *Nerve Agents*, Aberdeen Proving Ground, MD (Aug. 3); http://www.osha.gov/SLTC/emergencypreparedness/guides/nerve_cwa_air_table_08032004.pdf.

CHPPM, 2006, Chemical Warfare Agent Criteria, Summary Information, March 2006, http://usachppm.apgea.army.mil/chemical_agent/PDFFiles/ChemicalWarfareAgentCriteria_SummaryMar2006.pdf.

Codex (Codex Alimentarius Commission), 1999, *Submission of National Dietary Intake Data for 97.5% High Intake Consumers (by the United States),* March; as cited in Food Standards Australia New Zealand (FSANZ), 2000 (below).

Cyr, W.H., and B.F.J. Page, 2000, "EtO Residuals, A Guide to ISO 10993-7 and AAMI TIR-19 for EtO-Sterilized Devices," *Medical Device & Diagnostic Industry Magazine* (published Feb.); http://www.devicelink.com/mddi/archive/00/02/007.html.

Dahlke/DoD (U.S. Department of Defense), Undated, *The Terrorist NBC Threat: What We Are Up Against*, LTC Dale W. Dahlke, Ohio Military Reserve, NBC Defense School Commander, accessed 2006; http://www.sgaus.org/dahlke.htm.

DA (U.S. Department of the Army), 2004, I*mplementation guidance policy for revised airborne exposure limits for GB, GA, GD, GF, VX, H, HD and HT*. Washington, DC: Office of the Assistant Secretary (Installations and Environment), Department of the Army (June).

DoD, 1990, *Potential Military Chemical/Biological Agents and Compounds,* prepared by Headquarters Department of the Army (Field Manual 3-9), Department of the Navy (Publication No. P-467), Department of the Air Force (Manual 355-7), Washington, DC (Dec.); http://www.globalsecurity.org/wmd/library/policy/army/fm/3-9/fm3-9.pdf.

DoD, 2002, *Technical Report, Modeling and Risk Characterization of U.S. Demolition Operations at the Khamisiyah Pit*, Washington, DC (April 16); Appendix B III; http://www.gulflink.osd.mil/khamisiyah_tech/kham_tech_s18.htm.

DOE (U.S. Department of Energy) , 2005, *Revision 21 of AEGLs, ERPGs and TEELs for Chemicals of Concern*, Office of Environment, Safety, and Health, Washington, DC (Oct.); http://www.eh.doe.gov/chem_safety/ teel.html.

Elliot, S., G.E. Streit, J. Gaffney, J.E. Bossert, M. Brown, J. Reisner, and L.A. McNair, 1988, *Pathways for the Oxidation of (Sarin) in Urban Atmospheres*, LA-13501-MS, UC-700, prepared by Los Alamos Laboratory, Los Alamos, NM (Sept.); http://www.fas.org/sgp/othergov/ doe/lanl/lib-www/la-pubs/00418782.pdf.

Elliot, S., G.E. Streit, J. Gaffney, J.E. Bossert, M. Brown, J. Reisner, and L.A. McNair, 1989, "Pathways for the Oxidation of Sarin in Urban Atmospheres," *Environmental Science and Pollution Research*, 6(2):103–105.

Endo, A., Y. Yamaguchi, and K. F. Eckerman, 2005, *Nuclear Decay Data for Dosimetry Calculations – Revised Data of ICRP Publication 38*, Japan Atomic Energy Research Institute, JAERI 1347.

EPA 1988, Available online at http://www.epa.gov/iris/subst/0103.htm.

EPA (U.S. Environmental Protection Agency), 1989, *Risk Assessment Guidance for Superfund: Volume 1, Human Health Evaluation Manual (Part A),* EPA/540/1-89/002, Office of Emergency and Remedial Response, Washington, DC; http://www.epa.gov/oswer/riskassessment/ ragsa/index.htm.

EPA, 1990, Available online at http://www.epa.gov/iris for the following entries: Fenamiphos, Fenamiphos sulfoxide, and Formaldehyde.

EPA, 1991a, *Reregistration Eligibility Document (RED), Carbon and Carbon Dioxide*, Office of Pesticide Programs (Sept.); http://www.epa.gov/oppsrrd1/REDs/4019red.pdf.

EPA, 1991b, Guidance on implementing the radionuclide NESHAPS. USEPA Office of Radiation Programs. July 1991. Available online at http://www.epa.gov/rpdweb00/docs/neshaps/nesh_implement_07_91.pdf.

EPA, 1993, Available online at http://www.epa.gov/iris for the following entries: Dichlorvos, Methanol, Hydrogen cyanide, Red phosphorus, Phosphine, and Isopropyl methylphosphonic acid.

EPA, 1994, *Reregistration Eligibility Document, Boric Acid and Its Sodium Salts, List A, Case 0024*, Office of Pesticide Programs, Washington, DC (Feb. 16); http://www.epa.gov/oppsrrd1/REDs/old_reds/boric_acid_salts.pdf.

EPA, 1995a, *Reregistration Eligibility Decision (RED), Sodium Fluoroacetate, List C, Case 3073,* EPA 738-R-95-025, Office of Prevention, Pesticides and Toxic Substances, Washington, DC (Sept); http://www.fluoridealert.org/pesticides/Sodium_fluoroacetate.RED.95.pdf.

EPA, 1995b, Available online at http://www.epa.gov/IRIS/subst/0024.htm.

EPA, 1996, National Toxics Rule: Remand of Water Quality Criteria for Dioxin and Pentachlorophenol to EPA for Response to Comments. Federal Register Environmental Documents. *Federal Register*: December 11, 1996 (Volume 61, Number 239) http://www.epa.gov/fedrgstr/EPA-WATER/1996/December/Day-11/pr-21087.html.

EPA, 1997a, *Exposure Factors Handbook,* EPA/600/P-95/002F, Office of Research and Development, Washington, DC (Aug.); http://www.epa.gov/ncea/exposfac.htm.

EPA, 1997b, *National Ambient Air Quality Standards (NAAQS)*, Office of Air and Radiation, Washington, DC; http://www.epa.gov/air/criteria.html.

EPA, 1997c, *Registration Eligibility Decision (RED), Paraquat Dichloride,* EPA 738-F-96-018, Office of Prevention, Pesticides and Toxic Substances, Washington, DC (Aug.); http://www.epa.gov/oppsrrd1/REDs/0262red.pdf.

EPA, 1998a, *Registration Eligibility Decision (RED), Rodenticide Cluster*, EPA 738-R-98-007, Office of Prevention, Pesticides and Toxic Substances, Washington, DC (July); http://www.epa.gov/oppsrrd1/REDs/2100red.pdf.

EPA, 1998b, Table 3, *Chronic Toxicity of Pesticides Detected by the U.S. Department of Agriculture (USDA) Pesticide Data Program*, 1994 – 1998. http://ecologic-ipm.com/PDP/Table3_1998.pdf.

EPA, 1999a, *Human Health Risk Assessment, Fenamiphos,* Health Effects Division (7509C), Office of Pesticide Programs, Washington, DC (Sept. 2); http://www.epa.gov/pesticides/op/ fenamiphos/hedsep99.pdf.

EPA, 1999b, Cancer risk coefficients for environmental exposure to radionuclides. Federal Guidance Report No. 13, EPA 402-R -99-001. Prepared by Eckerman, K. F.; Leggett, R. W.; Nelson, C. B.; Puskin, J. S.; Richardson, A. C. B.

EPA, 2000b, *Report on FQPA Tolerance Reassessment Progress and Interim Risk Management Decision, Mevinphos*, EPA 738-R-00-014, Office of Prevention, Pesticides and Toxic Substances, Washington, DC (Sept.); http://www.epa.gov/oppsrrd1/REDs/0250tred.pdf.

EPA, 2000c, *Oxamyl (103801) Registration Case No. 0253; Revised Anticipated Residue and Acute and Chronic Dietary Exposure Estimates*, memorandum from J.S. Punzi to C. Jarvis, Health Effects Division, Office of Prevention, Pesticides and Toxic Substances, Washington, DC (March 9th); http://www.epa.gov/oppsrrd1/reregistration/oxamyl/acute.pdf.

EPA, 2000d, *IRED, Oxamyl*, EPA 738-R-00-015, Health Effects Division (7508C), Office of Prevention, Pesticides and Toxic Substances, Washington, DC (Oct.); http://www.epa.gov/oppsrrd1/REDs/0253ired.pdf.

EPA, 2000e, *Phosgene Hazard Summary* – Created in April 1992; Revised in January 2000, Fact Sheet on EPA's Technology Transfer Network Air Toxics Web site, Washington, DC (Jan.); http://www.epa.gov/ttn/atw/hlthef/phosgene.html.

EPA, 2000f, Report on FQPA Tolerance Reassessment Progress and Interim Risk Management Decision, Mevinphos, Office of Prevention, Pesticides and Toxic Substances, Washington, DC (Sept.); http://www.epa.gov/pesticides/reregistration/REDs/0250tred.pdf.

EPA, 2000g, National Primary Drinking Water Regulations; Radionuclides; Final Rule. Federal Register: December 7, 2000 (Volume 65, Number 236). 40 CFR Part 141 (65 FR 76708) Federal Register Environmental Documents.

EPA, 2001, *IRED for Phorate, List B, Case 0103*, Office of Prevention, Pesticides and Toxic Substances, Washington, DC; http://www.epa.gov/oppsrrd1/REDs/phorate_ired.pdf.

EPA, 2002b, *IRED, Fenamiphos*, EPA 738-R-02-004, Office of Prevention, Pesticides and Toxic Substances, Washington, DC (May); http://www.epa.gov/oppsrrd1/REDs/fenamiphos_ired.pdf.

EPA, 2002c, *Nicotine; Tolerance Revocations, Final Rule* (40 Code of Federal Regulations Part 180), *Federal Register* 67(99):35912–35915. July 1, Vol. 20; http://www.epa.gov/fedrgstr/EPA-PEST/2002/May/Day-22/p12423.htm.

EPA, 2003a, *Human Health Toxicity Values in Superfund Risk Assessments*, OSWER Directive 9285.7-53, Office of Solid Waste and Emergency Response, Washington, DC (Dec. 5); http://www.epa.gov/oswer/riskassessment/pdf/hhmemo.pdf.

EPA, 2003b, *IRED for Methyl Parathion*, Case No. 0153, Office of Prevention, Pesticides and Toxic Substances, Washington, DC (IRED signed May); http://www.epa.gov/oppsrrd1/REDs/methylparathion_ired.pdf.

EPA, 2004a, *2004 Edition of the Drinking Water Standards and Health Advisories (Winter 2004),* EPA 822-R-04-005, Office of Water, Washington, DC; http://www.epa.gov/waterscience/criteria/drinking/standards/dwstandards.pdf.

EPA, 2004b, *Drinking Water Health Advisory for Oxamyl*, EPA-822-B-04-002, Health and Ecological Criteria Division, Office of Science and Technology, Office of Water, Washington, DC (Sept.); http://www.epa.gov/waterscience/criteria/drinking/oxamyl-dw-ha.pdf.

EPA, 2004c, *Guidelines Establishing Test Procedures for the Analysis of Pollutants; Procedures for Detection and Quantitation*, 40 CFR Part 136; Office of Science and Technology; Office of Water; Washington, DC; Federal Register, 69(215):64704–7 (Nov. 8); http://www.epa.gov/fedrgstr/EPA-WATER/2004/November/Day-08/w24824.htm.

EPA, 2004d, *Users' Guide and Technical Background Document for U.S. EPA Region 9's Preliminary Remediation Goals (PRG) Table, Region 9: Superfund* (Dec. revision); http://www.epa.gov/region09/waste/sfund/prg/files/04usersguide.pdf.

EPA, 2004e, *Drinking Water; National Primary Drinking Water Regulations – Sulfate; National Primary Drinking Water Regulation Implementation*, *Federal Register* (Dec. 20); http://www.epa.gov/fedrgstr/EPA-WATER/1994/December/Day-20/pr-32DIR/fulltext.html.

EPA, 2004f, National Emission Standards for Hazardous Air Pollutants; National Emission Standards for Emissions of Radionuclides Other Than Radon from Department of Energy Facilities; National Emission Standards for Radionuclide Emissions from Federal Facilities Other Than Nuclear Regulatory Commission Licensees and Not Covered by Subpart H; Final Amendment—Correction. *Federal Register*: June 17, 2004 (Volume 69, Number 116). Federal Register Environmental Documents. http://www.epa.gov/fedrgstr/EPA-AIR/2004/June/Day-17/a13679.htm.

EPA, 2005a, *Standardized Analytical Methods for Use During Homeland Security Events,* Revision 2, Office of Research and Development, National Homeland Security Research Center, Cincinnati, OH (Sept.); http://www.epa.gov/nhsrc/pubs/reportSAM092905.pdf.

EPA, 2005b, *Provisional Peer-Reviewed Toxicity Values for Ammonia (CAS RN 7664-41-7),* Superfund Health Risk Technical Support Center, Office of Research and Development, National Center for Environmental Assessment, Cincinnati, OH; 2-2-05 (accessed electronically Nov.); http://hhpprtv.ornl.gov/ pprtv_papers.html.

EPA, 2005c, *Propylene Oxide – Revised HED Risk Assessment for Reregistration Eligibility Decision (RED)* , PC Code: 042501, DP Barcode: D321759, Office of Prevention, Pesticides, and Toxic Substances, Washington, DC (Sept. 26); http://cfpub.epa.gov/oppref/rereg/ status.cfm?show=rereg.

EPA, 2006a, Envirofacts Master Chemical Integrator, Chemical References Complete Index (accessed July 2006); http://www.epa.gov/enviro/html/emci/chemref/complete_index.html.

EPA, 2006b, *Integrated Risk Information System,* online database, Office of Research and Development, Washington, DC; http://www.epa.gov/iris. *Note: IRIS was accessed in November 2005 (with selected rechecks in January and July 2006), so the reference is presented here as 2006. However, dates in the tables represent when the chemical-specific toxicity values were placed online (or in some cases further reviewed), so that time frame can be appreciated when comparing with other benchmarks that may have been established earlier or later.*

EPA, 2006c, *Acute Exposure Guideline Levels for Ethyldichloroarsine,* OPPTS, OPPT, Washington, DC (March.); http://www.epa.gov/oppt/aegl/rest136.htm.

EPA, 2006d, *IRED for Dicrotophos,* (DDVP), Health Effects Division, Office of Prevention, Pesticides and Toxic Substances, Washington, DC (June); http://www.epa.gov/pesticides/reregistration/REDs/ddvp-ired.pdf.

EPA, 2006e, *Finalization of IRED for Phorate*. OPPTS, OPPT. Washington, DC (July); http://www.epa.gov/oppird1/reregistration/REDs/phorate.ired.pdf.

EPA, 2006f, *Drinking water contaminants.* http://www.epa.gov/safewater/contaminants/index.html.

EPA, 2006g, *IRED for Dicrotophos, Case No. 0145*, Office of Prevention, Pesticides and Toxic Substances, Washington, DC (July 31); http://www.epa.gov/oppsrrd1/REDs/dicrotophos_ired.pdf."

EPA, 2007a, *Standardized Analytical Methods for Environmental Restoration following Homeland Security Events*. Revision 3.0. Office of Research and Development, National Homeland Security Research Center, Cincinnati, OH.

EPA, 2007b, Memorandum: Use of Uranium Drinking Water Standards under 40 CFR 141 and 40 CFR 192 as Remediation Goals for Groundwater at CERCLA sites. From Elaine F. Davies, Acting Director, Office of Emergency and Remedial Response (OERR), and Stephen D. Page, Director, Office of Radiation and Indoor Air (ORIA), Office of Air and Radiation. Last updated on Friday, March 23rd, 2007. http://www.epa.gov/swerffrr/documents/uranium_drinking_water_standards.htm.

EPA Region 6, 2007, Region 6 Human Health Medium-Specific Screening Levels. Available online at http://www.epa.gov/earth1r6/6pd/rcra_c/pd-n/screenvalues.pdf.

Ershow, A. G., and K. P. Cantor, 1989, *Total Water and Tap Water Intake in the United States: Population Based Estimates of Quantities and Sources*, Order No. 263-MD-810264 (National Cancer Institute, Bethesda, MD).

Federal Register 56, July 18, 1991, U.S. Environmental Protection Agency. National Primary Drinking Water Regulations; Radionuclides; Proposed Rule. Vol. 56, No. 138, pp. 33050-33127 (Thursday, July 18, 1991).

Food Standards Australia New Zealand (FSANZ), 2000, *Full Assessment Report, MRL for Ethylene Oxide in Herbs and Spices, Application A412*, 10/01 (29 Nov.); http://www.foodstandards.gov.au/standardsdevelopment/applications/applicationa412useofethyleneoxideinherbsandspices/applicationa412fulla985.cfm.

FSANZ, 2002, *Final Assessment Report, Application A445, Maximum Residue Limits, Ethylene Oxide (s.37)*, 04/03 (9 Oct.); http://www.foodstandards.gov.au/_srcfiles/A445_FAR_091002.pdf.

IPCS (Industrial Programme on Chemical Safety), 1982, *Pesticide Residues in Food – 1982, Evaluations 1982 (Phorate)*; http://www.inchem.org/documents/jmpr/jmpmono/v82pr28.htm.

ICRP (International Commission on Radiological Protection), 1994, . *Human respiratory tract model for radiological protection*. ICRP Publication 66. Oxford: Pergamon Press.

ICRP, 1996, *Age-dependent doses to members of the public from intake of radionuclides. Part 5, Compilation of ingestion and inhalation dose coefficients.* ICRP Publication 72. Oxford: Pergamon Press.

IPCS, 1997, *Pesticide Residues in Food – 1997, Toxicological and Environmental Evaluations 1994, Fenamiphos*; http://www.inchem.org/documents/jmpr/jmpmono/v097pr06.htm.

Karpas, Z., A. Lorber, H. Sela, O. Paz-Tal, Y. Hagag, P. Kurttio, L. Salonen, 2005, Measurement of the ^{234}U / ^{238}U ratio by MC-ICPMS in drinking water, hair, nails, and urine as an indicator of uranium exposure source. *Health Phys.* 89: 315–321.

Kimmell, T., 2005, *Sources of Uncertainty in Sampling Laboratory Analytical Methods for 15 Priority Threat Chemicals in Air and Water (Draft)*, prepared by Environmental Assessment Division, Argonne National Laboratory for EPA, Office of Research and Development, National Homeland Security Research Center (Nov. 25).

MacDonell, M., A. Davidson, K. Picel, and J. Peterson, 2005, *Summary Detection Information for the Initial Study Contaminants in Water, Integrated Management Summary (Draft)*, prepared by Environmental Assessment Division, Argonne National Laboratory for EPA, Office of Research and Development, National Homeland Security Research Center (Aug. 12).

Maui DOWS (Department of Water Supply), 2004 (1999-2004), *Lead and Phosphates*, prepared by Department of Water Supply, Maui, HI; http://mauiwater.org/phosphates.html.

McDowell, M. A., R. D. Briefel, K. Alaimo, A. Bischof, C. Caughman, M. Carroll, C. Loria, C. Johnson, 1994, *Energy and Macronutrient Intakes of Persons Ages 2 Months and Over in the United States: Third National Health and Nutrition Examination Survey, Phase 1, 1989 91*, Advance Data 255 (U. S. Dept. of Health and Human Services).

MDCH (Michigan Department of Community Health), 2006 (accessed), *Toxic Substances Fact Sheet (Hydrogen Sulfide)*; http://www.michigan.gov/documents/hydrogensulfide_factsheet__6538_7.pdf.

Mitretek, 2005, *Chemistry of L (Lewisite)*, Falls Church, VA;
http://www.mitretek.org/ ChemistryOfLLewisite.htm.

Munro, N., S.S. Talmage, G.D. Griffin, L.C. Waters, A.P. Watson, J.F. King, and V. Hauschild, 1999, "The Sources, Fate, and Toxicity of Chemical Warfare Agents Degradation Products," *Environmental Health Perspectives,* 107(12):933–974 (Dec.);
http://ehp.niehs.nih.gov/members/1999/107p933-974munro/munro-full.html.

NAS (National Academy of Sciences), 1999, *Review of the U.S. Army's Health Risk Assessments for Oral Exposure to Six Chemical-Warfare Agents,* National Academies Press, Washington, DC; http://darwin.nap.edu/books/0309065984/html/R1.html.

NAS, 2000a, *Organic Phosphonates,* Chapter 14 in *Toxicological Risks of Selected Flame-Retardant Chemicals*, National Academies Press, Washington, DC;
http://www.nap.edu/books/ 0309070473/html/307.html.

NAS, 2000b, *Strategies to Protect the Health of Deployed U.S. Forces: Detecting, Characterizing, and Documenting Exposures,* National Academies Press, Washington, DC;
http://www.nap.edu/books/0309068754/html.

NAS, 2004, *Emergency and Continuous Exposure Guidance Levels for Selected Submarine Contaminants,* National Academies Press, Washington, DC;
http://darwin.nap.edu/books/0309092256/html.

NRC (National Research Council), 1997, "Red phosphorous smoke," Chapter 4, pp 98–126 in *Toxicity of Military Smokes and Obscurants*, Vol 1. Committee on Toxicology, Subcommittee on Military Smokes & Obscurants. National Academy Press, Washington, DC.

NRC, 2003, "Nerve agents GA, GB, GD, GF and VX," Chapter 1, pp 15–300, and "Sulfur Mustard", Chapter 2, pp. 301–383 in *Acute Exposure Guideline Levels for Selected Airborne Chemicals*, Vol 3. Committee on Toxicology, Subcommittee on Acute Exposure Guideline Levels. The National Academy Press, Washington, DC.

NCHS (U. S. Department of Health and Human Services), 1992, *Vital Statistics Mortality Data*, *Detail, 1989,* NTIS order number for datafile tapes: PB92 504554 (Public Health Service, National Center for Health Statistics, Hyattsville, MD).

NCHS, 1993a, *Vital Statistics Mortality Data*, *Detail, 1990,* NTIS order number for datafile tapes: PB93 504777 (Public Health Service, National Center for Health Statistics, Hyattsville, MD).

NCHS, 1993b, *Vital Statistics Mortality Data*, *Detail, 1991,* NTIS order number for datafile tapes: PB93 506889 (Public Health Service, National Center for Health Statistics, Hyattsville, MD).

NCHS, 1997, U. *S. Decennial Life Tables for 1989–91*, Vol. 1, No. 1. DHHS, PHS-98-1150-1 (United States Life Tables. Public Health Service, Washington, DC). October, 1997.

NZERMA (New Zealand Environmental Risk Management Authority), 2003, *Draft Tolerable Exposure Limits, Hydrogen Cyanide, Chloropicrin, Phosphine, 1,3-Dichloropropene, Methyl Bromide (Appendix 2).*

NZFSA (New Zealand Food Safety Authority), 2005, *New Zealand (Maximum Residue Limits of Agricultural Compounds) Food Standards 2005, WTO Consultation: Amendment Two: May/June 2005* (July 25); http://www.nzfsa.govt.nz/policy-law/legislation/food-standards/nz-food-standards-2005-mrl-no-2.pdf.

Opresko, D.M., et al., 1998, "Chemical Warfare Agents: Estimating Oral Reference Doses," *Reviews of Environmental Contamination & Toxicology*, 156:1–183. Abstract available at http://www.ncbi.nlm.nih.gov/ entrez/query.fcgi?cmd=Retrieve&db=PubMed&list_uids=9597943&dopt=Abstract.

Opresko, D. M., R. A. Young, A. P. Watson, et al., 2001, Chemical Warfare Agents: Current status of oral reference doses. *Rev. Environ. Contam. Toxicol.* 172:65-85.

Patocka, J., and J. Bajgar, 1998, *Toxicology of Perfluoroisobutylene*, ASA Newsletter, ISSN 1057-9419; http://www.asanltr.com/ASANews-98/pfib.html.

Peterson, J., M. MacDonell, L. Haroun, and F. Monette, 2005, *Radiological and Chemical Fact Sheets to Support Health Risk Analyses for Contaminated Areas*, prepared in collaboration with R.D. Hildebrand, U.S. Department of Energy, Richland Operations Office, and A. Taboas, DOE Chicago Operations Office, by Argonne National Laboratory, Environmental Science Division, Argonne, IL (Aug.); http://www.ead.anl.gov/pub/dsp_detail.cfm?PubID=1472.

Picel, K., M. MacDonell, A. Davidson, J. Peterson, S. Collie, S. Garcia, and A. Johns, 2005a, *Summary Detection Information for the Initial Study Contaminants in Air (Draft)*, prepared by Environmental Assessment Division, Argonne National Laboratory, and Tetra Tech EM Inc. for U.S. Environmental Protection Agency, Office of Research and Development, National Homeland Security Research Center (Jun. 5).

Picel, K., M. MacDonell, A. Davidson, J. Peterson, S. Collie, S. Garcia, and A. Johns, 2005b, *Summary Detection Information for the Initial Study Contaminants in Water (Draft)*, prepared by Environmental Assessment Division, Argonne National Laboratory, and Tetra Tech EM Inc. for U.S. Environmental Protection Agency, Office of Research and Development, National Homeland Security Research Center (Aug. 12).

Putnam, J.J., and J.E. Allshouse, 1999, *Food Consumption, Prices, and Expenditures, 1970–97*, Statistical Bulletin No. 965, Food and Rural Economics Division, Economic Research Service, USDA, Washington, DC (April); http://www.ers.usda.gov/publications/sb965/.

Rae Systems, 2003, *Chemical Warfare Measurements by PID*, Technical Note TN-159, Sunnyvale, CA (Oct.); http://www.raesystems.com/~raedocs/App_Tech_Notes/Tech_Notes/TN-159_Nerve_Agents_by_PID.pdf.
Reddy, G. G., A.A. Major and G.J. Leach. 2005. Toxicity Assessment of Thiodiglycol. *Internat. J. Toxicol.* 24:435–442.

Rega, P.P., E. Mowatt-Larssen, and D.P. Sole, 2006, *CBRNE – Irritants: Cs, Cn, Cnc, Ca, Cr, Cnb, PS*, prepared for eMedicine (April); http://www.emedicine.com/emerg/topic914.htm.

RI (Rhode Island), 2004, *Rhode Island Air Toxics Guideline* (April); http://www.dem.ri.gov/programs/benviron/air/pdf/airtoxgl.pdf.

Syracuse Research Corporation (SRC), 2006, *Environmental Fate Data Base*, online database (accessed 2006), Syracuse, NY; http://www.syrres.com/esc/efdb.htm.

Talmage, S. S., N. B. Munro, A. P. Watson, et al., 2007, "The Fate of Chemical Warfare Agents in the Environment." Chapt 4, pp 89–125 in T. C. Marrs, R. L. Maynard and F. R. Sidell (eds), *Chemical Warfare Agents: Toxicology and Treatment, 2nd Edition*, John Wiley & Sons, Ltd. West Sussex, England.

Watson, A. P. and F. G. Dolislager, 2007, *Reevaluation of 1999 Health –Based Environmental Screening Levels (HBESLs) for Chemical Warfare Agents*. ORNL/TM-2007/080. Oak Ridge National Laboratory, Oak Ridge, TN 37830.

WIDHFS (Wisconsin Department of Health & Family Services), 2004, *Gasoline*, toxic chemical fact sheet (last revised Dec.); http://dhfs.wisconsin.gov/eh/ChemFS/fs/Gasoline.htm.

Wong, C.T., H. Okamoto, A. Milea, S. Perera, F. Baumann, 1999, Isotopic uranium activity ratios in California groundwater. *J. Amer. Water Works Assoc.* 91: 171–185.

A Appendix A: Supporting Details for Overall Approach and Key Benchmarks

This appendix includes two figures (A1 and A2) that illustrate a general process for identifying risk-based target concentrations to help guide detection validation. One table is also provided to support the analyses in the main body of this report, as described below.

Table A1:	Illustrates further details for eight types of drinking water benchmarks, six based on concentrations and two on dose values. (This table is adapted from the summary in the recent standards and guidelines report for the NHSRC-ANL pilot drinking water study.) This information provides background context for the applicability of various benchmarks to support target concentrations for detection validation.

Figure A1 **Fate Evaluation to Identify Associated Chemicals for Detection Consideration, and Overview Benchmark Check**

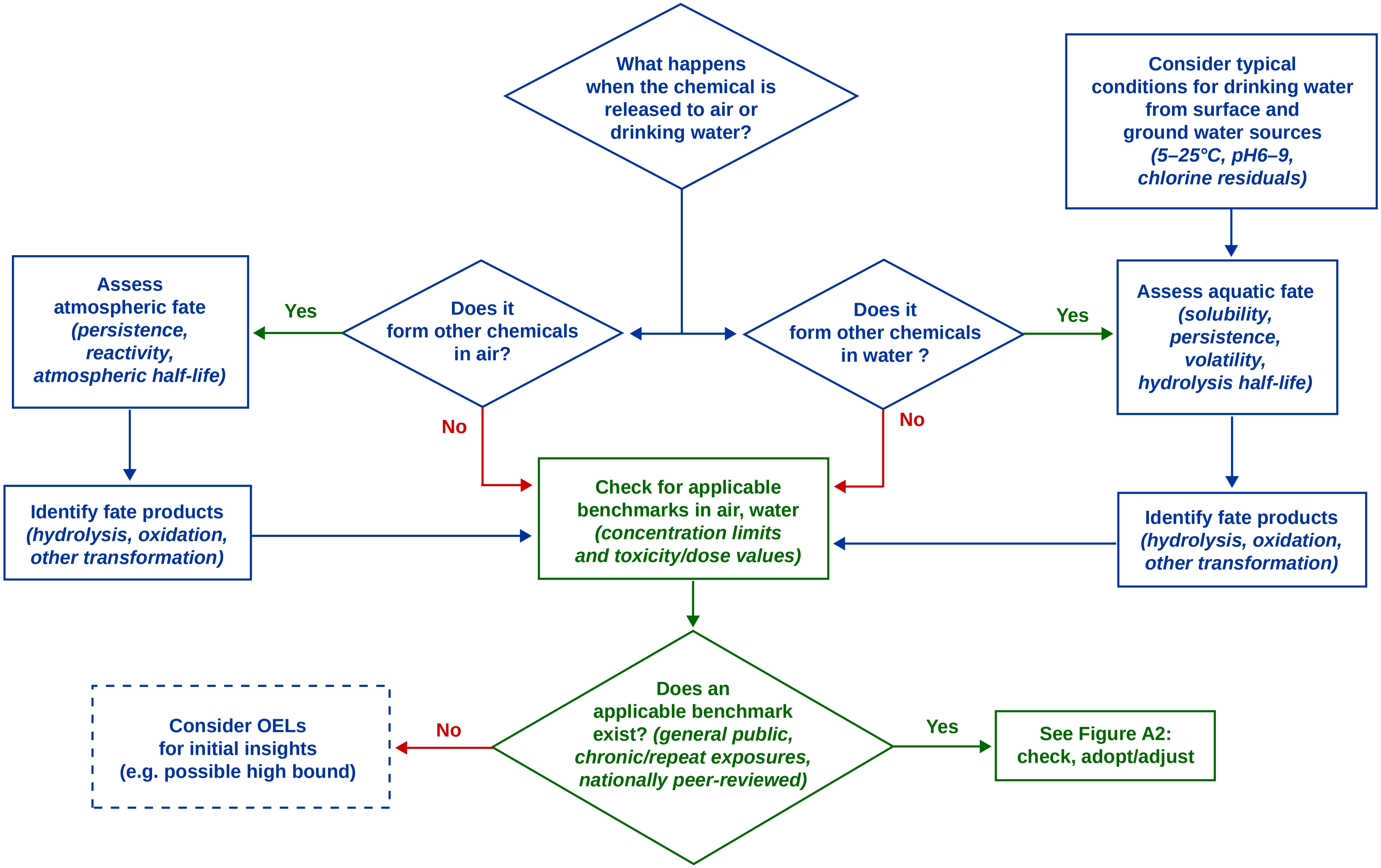

Figure A2 **Example Evaluation Process for Chronic Concentrations**

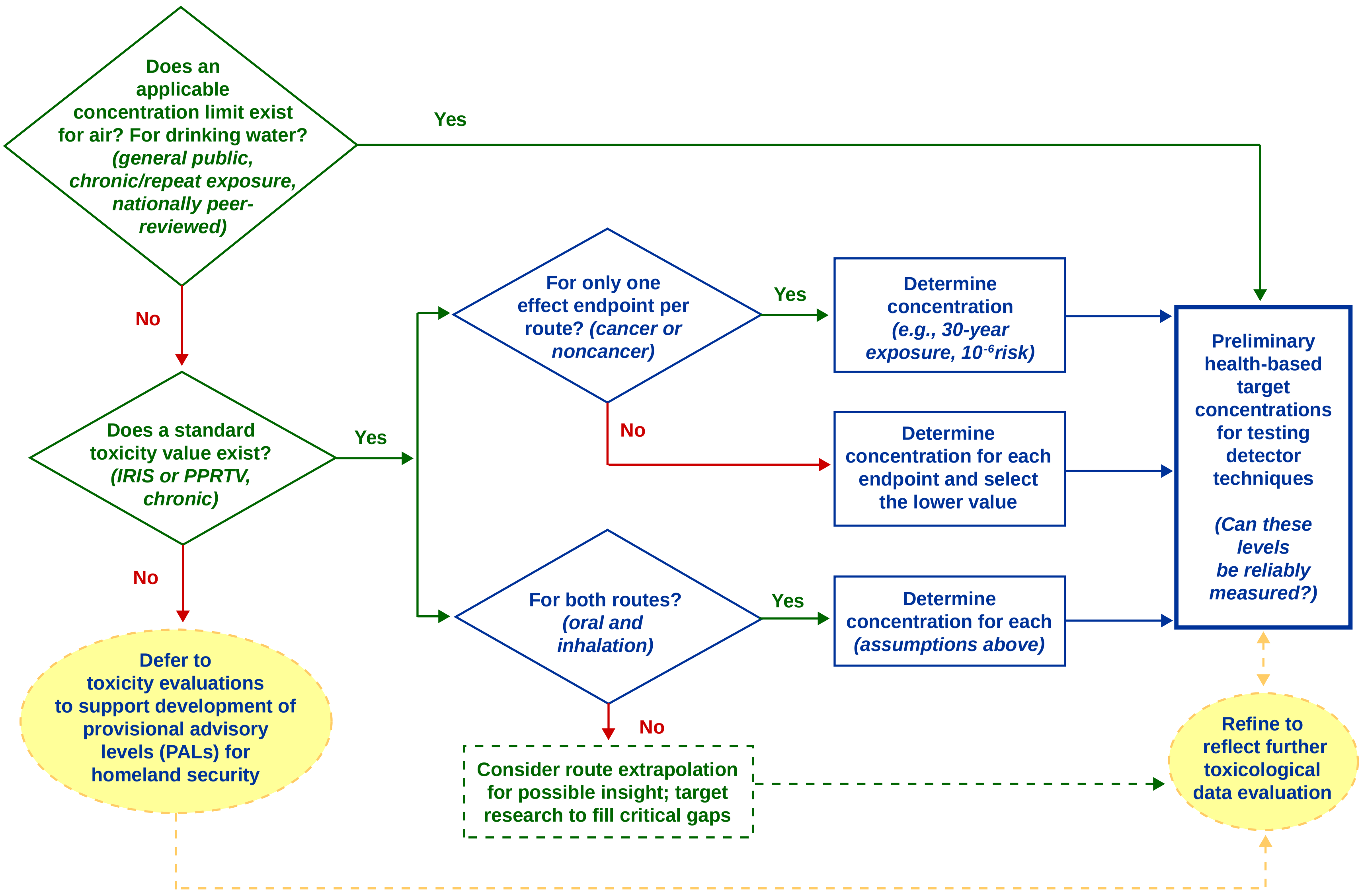

Table A1 Overview Description of Exposure Criteria and Dose Benchmarks for Drinking Water[a]

Standard/Guideline and Organization	Summary Description	Target Group	Exposure Parameters Assumed			Example of Chemicals Covered
			Duration	Body Weight/ Age	Intake Rate	
Maximum contaminant level (MCL) *EPA Office of Water*	Enforceable concentration for public water supplies, aims to protect the population	General public	Chronic/lifetime	70-kg adult	2 L/d	Arsenic, asbestos, carbofuran, cyanide, fluoride, mercury
Minimal risk level (MRL) *Agency for Toxic Substances and Disease Registry*	Dose level based on NOAEL for noncancer effects (MRLs also exist for shorter exposure durations)	General public	Acute (1–14 d)	70-kg adult	2 L/d	Arsenic, cyanide, dichlorvos, DIMP, formaldehyde, methyl parathion
			Intermediate (15–364 d)			
			Chronic (≥1 yr)			
Drinking water equivalent level (DWEL) *EPA Office of Water*	No-effect concentration from multiplying the oral RfD by an adult body weight and dividing by the daily intake	General public	Chronic/lifetime	70-kg adult	2 L/d	Arsenic, carbofuran, cyanide, cyanogen chloride, DIMP, methyl parathion
Health advisory (HA) *EPA Office of Water*	Concentration in drinking water to not produce any adverse noncancer effects	General public	Acute (1 d, 10 d)	10-kg child	1 L/d	Ammonia, cyanide, IMPA, methyl parathion, oxamyl
			Chronic/lifetime	70-kg adult	2 L/d	
Drinking water level of comparison (DWLOC) *EPA OPP*	Concentration as portion of pesticide exposure from drinking water to not cause any adverse noncancer effects	General public	Acute (1 d), short-term (to 7 d), intermediate (3 month [mo]), chronic (lifetime)	10-kg infant, child	1 L/d	Dicrotophos, fenamiphos, methyl parathion
				60-kg adult female, 70-kg adult male	2 L/d	
Oral RfD *EPA ORD (IRIS)*	Estimate of daily oral exposure (dose) likely to be without appreciable risk of adverse noncancer effect over a lifetime (including for susceptible subgroups)	General public	Chronic/lifetime	70-kg adult	2 L/d	Aldicarb, carbofuran, carbon disulfide, dicrotophos, furan, methyl parathion, paraquat, phenol, phosphine, strychnine
Cancer slope factor (SF) and UR *PA ORD (IRIS)*	Plausible upper-bound probability individual will develop cancer as a result of exposure (dose) over lifetime	General public	Chronic/lifetime	70-kg adult	2 L/d	Arsenic, benzene, 1,2-dichloroethane, dichlorvos, PCBs, propylene oxide
Military exposure guideline (MEG) *U.S. Army CHPPM*	Operational concentration for moderate and arid climates to produce minimal to no adverse effects, can adjust for public	Deployed military personnel	< 7 d, 7–14 d	70-kg adult	5, 15 L/d	Carbofuran, carbon disulfide, cyanide, methyl parathion, oxamyl, paraquat
			1 yr			

[a] Examples illustrate several chemicals for which these benchmarks exist. Note that the levels identified for chronic (lifetime) exposures for the general public (e.g., MCL, RfD, and SF) incorporate consideration of children. DIMP = diisopropyl methylphosphonate; IMPA = isopropyl methylphosphonic acid; PCBs = polychlorinated biphenyls.

EPA/600/R-08/021 | October 2008 | www.epa.gov/ord

SC
IEN
CE

United States
Environmental Protection
Agency

Office of Research and Development
National Homeland Security Research Center
Cincinnati, OH 45268