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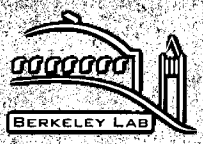

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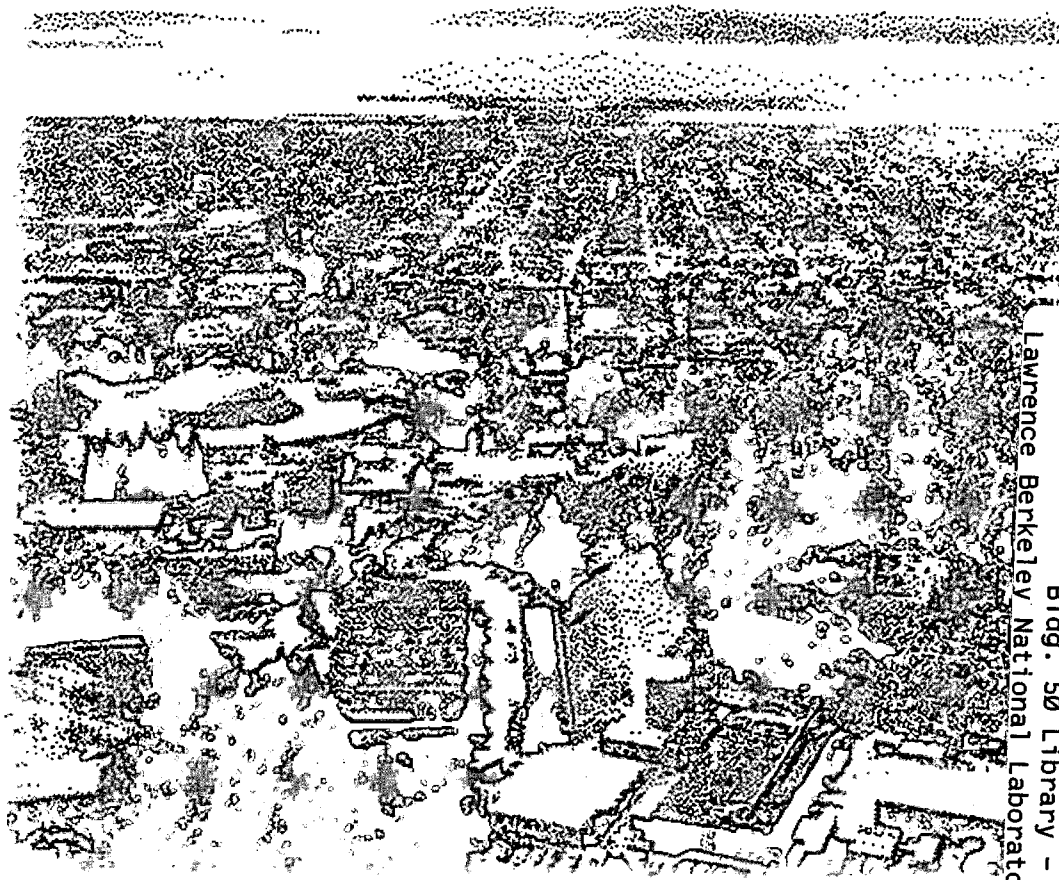
BERKELEY NATIONAL LABORATORY

Database of Physical, Chemical and Toxicological Properties of Chemical and Biological (CB) Warfare Agents for Modeling Airborne Dispersion In and Around Buildings

Tracy Thatcher, Rich Sextro, and Don Ermak

Environmental Energy Technologies Division

June 2000



DISCLAIMER

Database of Physical, Chemical and Toxicological Properties of Chemical and Biological (CB) Warfare Agents for Modeling Airborne Dispersion In and Around Buildings

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Purpose

The purpose of this report is to provide a single, consistent set of unclassified data on the physical, chemical and toxicological properties of chemical and biological (CB) agents that might be released in an urban terrorism incident, and references for the sources of the data. These data are needed for predicting airborne concentrations of CB agents in and around buildings as a function of time and their potential toxicological consequences, and for developing mitigation plans. As new information emerges, we will update this reference document. In addition to the data tables, Appendix A summarizes definitions and units for airborne concentrations of CB agents and related conversion factors and Appendix B presents more detailed information on the lethal dose and exposure levels for anthrax and sarin.

Background

The agents in this reference have been divided into two major classes: chemical and biological. The chemical agents have been further divided into sub-categories reflecting their toxicological effects, e.g., respiratory agents, nerve agents, etc. The biological agents are sub-divided into categories based on type of micro-organism. Within the sub-categories, agents are listed alphabetically.

Chemical and biological agents differ significantly in their physical forms and physical behavior in indoor and outdoor air. The chemical agents, such as phosgene or sarin, may be gases, liquids or solids at typical indoor conditions. The liquids may be dispersed as vapors and/or aerosols (droplets or particles). If dispersed as an aerosol, some of the liquid chemical agent may volatilize over time to give a mixture of vapor and particles. Chemical agents that are solids are often dispersed as powders, i.e., particles suspended in air. Vapors and particles exhibit different physical behavior with respect to persistence in air and deposition to surfaces.

In the first set of tables, the common and official chemical names of chemical agents are provided along with their Chemical Abstract Service (CAS) Registry numbers. The database includes molecular weight (MW), density, boiling and melting points, vapor pressure, vapor density and information on hydrolysis rate and solubility in water. Toxicological properties include the Airborne Exposure Limit (AEL), which is the 8-hour time-weighted concentration in air that is a permissible exposure, LCt_{50} , the exposure (in units of mg-min/m^3) at which death will occur in 50% of the exposed population, and the detoxification rate (if any).

Biological agents, listed in the second set of tables, are particles (aerosols), with sizes that vary depending upon the specific agent. They may consist of a toxin from a biological agent (e.g., botulinum toxin), a bacterial organism, (e.g., anthrax), a fungal agent (e.g., Valley fever), a rickettsia organism (e.g., typhus) or a viral organism (e.g., dengue fever). This document provides information on biological agents in each of these classes, on dissemination and/or route of exposure, range of particle size and shape, incubation period, contagiousness, and persistence. The particle size range represents the physical size of the organism or spore and, therefore, is the minimum particle size for an aerosol containing the agent. Actual particle size distributions for an aerosol containing a given biological agent will vary, depending primarily upon the preparation and dissemination methods. Thus, the mass median aerosol diameter and size distribution may be larger than the values given in Table 2A.

TABLES FOR CHEMICAL WARFARE AGENTS

Table 1A: Chemical Warfare Agents

Agent Type	Common Name[a]	Chemical Name	Code	CAS Number
Respiratory Agents	Chlorine	Chlorine		7782-50-5
	Diphosgene	Trichloromethyl chloroformate	DP	503-38-8
	Phosgene	Carbonyl chloride	CG	75-44-5
Nerve Agents	Sarin	Isopropylmethylphosphonofluoridate	GB	107-44-8
	Soman	Pinacolylmethylphosphonofluoridate	GD	96-64-0
	Tabun	Ethyl-n-dimethylphosphoroamidecyanidate	GA	77-81-6
	V-agents	Ethyl S-2 diisopropylaminoethyl-methylphosphonothioate	VX	50782-69-9
Blood Agents	Arsine	Arsenic trihydride	SA	7784-42-1
	Cyanogen Chloride	Cyanogen chloride	CK	506-77-4
	HCN	Hydrogen cyanide	AC	74-90-8
Blister Agents	Ethyldichloroarsine	Ethyldichloroarsine	ED	598-14-1
	Lewisite	Dichloro (2-chlorovinyl)arsine	L	541-25-3
	Methyldichloroarsine	Methyldichloroarsine	MD	593-89-5
	Mustard, Distilled	2,2- dichloro-diethyl-sulfide	HD	505-60-2
	Mustard-Lewisite	mix of HD and L	HL	
	Mustard-T Mixture	60% HD, 40% TT (similar to HD)	HT	
	Mustard, Nitrogen	2,2-dichloro-triethylamine	HN-1	538-07-8
	Mustard, Nitrogen	2,2,2-trichloro-triethylamine	HN-3	555-77-1
	Mustard, Sulfur	1,1- thiobis(2-chloroethane)	H	
	Phenyldichloroarsine	Phenyldichloroarsine	PD	696-28-6
	Phosgene Oxime	Dichloroformoxime	CX	1749-86-1
Vomiting Agents	Adamsite	Diphenylaminochloroarsine	DM	578-94-9
	Diphenylchloroarsine	Diphenylchloroarsine	DA	712-48-1
	Diphenylcyanoarsine	Diphenylcyanoarsine	DC	23525-22-6

a. When no common name is available, the chemical name is used.

Table 1B: Physical Properties of Chemical Warfare Agents (references indicated by numerical superscripts)

Common Name	Code	MW	Density (g/cc)	Boiling Point (°C)	Melting Point (°C)	Vapor Pressure (mmHg)	Vapor Density (air=1)	Hydrolysis	Solubility (in water)
Respiratory Agents									
Chlorine		71	1.41[1]	-34.5[1]	-101[1]	4992 (20)[1]	2.4[1]	Slow[1]	
Diphosgene	DP	198	1.65[1]	127[1]	-57[1]	4.2 (20)[1]	6.8[1]	Slow[1]	
Phosgene	CG	99	1.37[1]	7.6[1]	-128[1]	1173 (20)[1]	3.4[1]	Rapid[1]	
Nerve Agents									
Sarin	GB	141	1.09[1,2]	158[1,2]	-50[1]/-56[2]	2.9 (25)[1,2]	4.9[1,2]		Miscible[2,3]
Soman	GD	182	1.02[1,2]	198[1]	-42[1,2]	0.40 (25)[1,2]	6.3[1,2]	Slow[1]	2.10%[2,3]
Tabun	GA	162	1.07[1]	220[2]	-50[1,2]	0.07 (25)[1]	5.6[1,2]	Slow[1]	9.80%[3]
V-agents	VX	267	1.01[1,2]	298[1,2]	-51[1,2]	0.0007 (25)[1,2]	9.2[1,2]	Slow[1]	Slight[2]/Miscible[3]
Blood Agents									
Arsine	SA	78	1.34[1]	-62.5[1]	-116[1]	11100 (20)[1]	2.7[1]	Rapid[1]	
Cyanogen Chloride	CK	61	1.18[1]	13[1]	-7[1]	1000 (25)[1]	2.1[1]	Very slow[1]	6.90%[3]
HCN	AC	27	0.69[1]	26[1]	-13[1]	742 (25)[1]	0.9[1]	Low[1]	Complete[3]
Blister Agents									
Ethyldichloroarsine	ED	175	1.66[1]	156[1]	-65[1]	2.09 (20)[1]	6.0[1]	Rapid[1]	
Lewisite	L	207	1.89[1,2]	190[1,2]	0[1]	0.394 (20)[1,2]	7.1[1,2]	Rapid[1]	Insoluble[2]
Methyldichloroarsine	MD	161	1.84[1]	133[1]	-55[1]	7.76 (20)[1]	5.5[1]	Very Rapid[1]	
Mustard, Distilled	HD	159	1.27[1,2]	217[1,2]	14.5[1,2]	0.072 (20)[1,2]	5.4[1]/5.5[2]	17 min[1]	0.09%[3]
Mustard-Lewisite	HL	186	1.66[1]	190[1]	-25[1]	0.248 (20)[1]	6.5[1]	Slow[1]	
Mustard-T Mixture	HT								
Mustard, Nitrogen	HN-1	170	1.09[1]	194[1]	-34[1]	0.24 (20)[1]	5.9[1]	Slow[1]	
Mustard, Nitrogen	HN-3	205	1.24[1]	256[1]	-3.7[1]	0.0109 (25)[1]	7.1[1]	Slow[1]	
Mustard, Sulfur	H		1.24[3]	Varies[3]		Varies[3]	5.5[3]		0.09%[3]
Phenyldichloroarsine	PD	223	1.65[1]	252[1]	-20[1]	0.033 (25)[1]	7.7[1]	Rapid[1]	
Phosgene Oxime	CX	114	1.50[1]	54[1]	40[1]	None[1]	(solid)	Unknown[1]	70%[3]
Vomiting Agents									
Adamsite	DM	278	1.65[1]	410[1]	195[1]	2e-13 (20)[1]	(solid)	Rapid[1]	
Diphenylchloroarsine	DA	265	1.39[1]	333[1]	41[1]	0.0036(45)[1]	(solid)	Rapid (gas)[1]	
Diphenylcyanoarsine	DC	255	1.33[1]	350[1]	31.5[1]	0.0002 (20)[1]	(solid)	Moderate[1]	

Table 1C: Toxicological Properties of Chemical Warfare Agents (references indicated by numerical superscripts)

Common Name	Code	AEL[a] (mg/m^3)	LCt_{50} (inhalation)[b] (mg-min/m^3)	Detoxification Rate[c]
Respiratory Agents				
Chlorine			19000[1]	Rapid[1]
Diphosgene	DP		3200[1]	Negligible Detoxification[1]
Phosgene	CG		3200[1]	Negligible Detoxification[1]
Nerve Agents				
Sarin	GB	0.0001[2,6]	70[1,2], 100[3]	Slow[1]
Soman	GD	0.00003[2]	100[1], 70[2], 50[6]	Slow[1]
Tabun	GA	0.0001[2,6]	400[1,3], 135-400[6]	Slight[1]
V-agents	VX	0.00001[2,6]	100[1], 30[2], 10[3], 20-50[6]	Very Slow[1]
Blood Agents				
Arsine	SA		5000[1]	Slow[1]
Cyanogen Chloride	CK		11000[1,3]	Rapid[1]
HCN	AC		2000-5000[1,3]	Rapid[1]
Blister Agents				
Ethyldichloroarsine	ED		3000[1]	Rapid[1]
Lewisite	L	0.003[2]	1200-1500[1,2,3]	Negligible Detoxification[1]
Methyldichloroarsine	MD		3000[1]	Rapid[1]
Mustard, Distilled	HD	0.003[2,6]	1500[1,3], 10000[6]	Very Slow[1]
Mustard-Lewisite	HL		1500[1]	Negligible Detoxification[1]
Mustard-T Mixture	HT	0.003[6]	10000[6]	
Mustard, Nitrogen	HN-1		1500[1]	Negligible Detoxification[1]
Mustard, Nitrogen	HN-3		1500[1]	Negligible Detoxification[1]
Mustard, Sulfur	H	0.003[6]	1500[3], 10000[6]	
Phenyldichloroarsine	PD		2600[1]	Rapid[1]
Phosgene Oxime	CX		3200[3]	Very Slow[1]
Vomiting Agents				
Adamsite	DM		15000[1]	1-2 hrs[1]
Diphenylchloroarsine	DA		15000[1]	1-2 hrs[1]
Diphenylcyanoarsine	DC		10000[1]	1 hr[1]

[a] Airborne Exposure Limit: permissible 8 hour time weighted average concentration.

[b] Inhalation exposure which would be lethal for half of the exposed population.

[c] Rate at which the human body can metabolize or eliminate the toxin. Compounds with low detoxification rates may accumulate to dangerous level within the body, even at very low concentrations.

TABLES FOR BIOLOGICAL WARFARE AGENTS

Table 2A: Physical Properties of Biological Warfare Agents (references indicated by numerical superscripts)

Type	Common Name	Biological Class	Spore Forming	Persistence	Size (µm) [a.]	Shape
Biotoxins	Aflatoxins		NA		b.	
	Botulinus	otulinum toxin, protein	NA	12 hrs air[7]	b.	
	Ricin		NA	very stable[7]	b.	
	Tricothecene	anoprotein	NA	very stable[7]	b.	
Bacteria	Anthrax	acillus anthracis	2 hrs[1]	years[4]	~1 x ~1.5[12]	Rod[1,4]
	Brucellosis	rucella melitensis, abortus, and suis	No[1]			Rod[1]
	Cholera	ibrio cholera	No[4]			Bent Rod[4]
	Diptheria	orynebacterium Diptheriae	No[4]		0.5 to 1 (D) x 2 to 7 L)[4]	Curved Rod[4]
	Dysentary	higella Dysenteria	No[4]			Rod[4]
	Glanders	alleomyces Mallei	No[4]	2-3 weeks[4]		Rod[1,4]
	Melioidosis (Whitmore's)	alleomyces Pseudomallei	No[4]	month or more[4]	0.5 (D) x 1 to 2 (L) [4]	Rod[4]
	Paratyphoid Fever	almonella Paratyphi/Schottmuelleri	No[4]	weeks to months[4]		Short rod[4]
	Plague	asteurella Pestis	No[4]	days-weeks[4]		Rod[1,4]
	Pulmonary Tuberculosis	ycobacterium Tuberculosis		weeks to months[4]	.2 to 0.5 (D) x 1 to 4 (L)[4]	Slender rod[4]
	Salmonella food poisoning	almonella typhimurium	No[4]		0.5 (D) x 1 to 1.5 (L) [4]	Plump Rod[4]
	Tularemia	asteurella Tularensis	No[4]		varies[4]	Sphere[1]
	Typhoid Fever	almonella Typhosa	No[4]	weeks to months[4]		Rod[4]
Fungi	Histoplasmosis	istoplasma capsulatum	Yes[4]	months to years[4]	1 to 5[4]	Oval[4]
	Nocardiosis	ocardia Asteroides			diam <1[4]	Filament[4]
	Valley Fever	occidioides immitis	Yes[4]	months to years[4]	20 to 80[4]	Spherical[4]
Rickettsia	Endemic Typhus	ickettsia mooseri	NA			
	EpidemicTyphus	ickettsia prowazekii	NA		0.3[4]	Sphere/Rod[4]
	Q fever	oxiella burnetti	NA	5-60 days[4]	0.25 x 0.5 (D) to 1.5 (L)[4]	
	Scrub Typhus	ickettsia Tsutsugamushi	NA		0.2(D) x 0.4(L) to 0.5(D) x 1.3(L)[4]	Short Rods[4]
	Spotted fever	ickettsia rickettsii	NA		0.2 to 0.3 (D) x 1 (L) [4]	Rod Pairs[4]
Viruses	Denegue fever	enegue fever virus	NA		0.017 to 0.025[4]	
	Encephalitis	ncephalomyelitis viruses	NA	variable[4]		
	Influenza	nfluenza virus	NA		0.07 to 0.1[4]	
	Psittacosis		NA			
	Rift Valley fever		NA		0.023 to 0.035[4]	
	Smallpox	ariola virus	NA	years[4]	0.15 to 0.2[4]	
	Yellow fever	ellow fever virus	NA		0.017 to 0.028[4]	

a. For the sizes of rod shape biological agents, the diameter (D) and length (L) of the rod are given.
b. The biotoxins are chemicals produced by biological organisms; particle size will depend upon methods of preparation and dissemination.

Table 2B: Toxicological Properties of Biological Warfare Agents

Common Name	Dissemination/Route of Entry	Incubation/ Onset	Contagious?	50% Infective Dose (organisms/person)	Untreated Lethality (%)
Biotoxins					
Aflatoxins	Incapacitating or additive to other agents[1]		No		
Botulinus	Ingestion, contact with wounds, possibly inhalation[1,4]	6 hrs-8 days[1]	No	0.4 μg/person (LD_{50})[5]	
Ricin	Injection (umbrella, balls), microencapsulation[1]	hours[1]	No	0.1 mg/kg (LD_{50})[5]	
Tricothecene	Yellow-green powdered aerosol, encapsulation not required[1]		No	500 μg/kg (LD_{50})[7]	
Bacteria					
Anthrax (N)	Spore inhalation, ingestion (rare), broken skin[1,4]	1-2 hrs[1], 1-7 days[4]	No[5]	8,000 to 20,000[5]	100[5]
Brucellosis (US)	Broken skin, eyes, ingestion[1]	1-3 wks[1], 1-8.5 wks[2]	No[4]		2[1]
Cholera	Ingestion, flies[1]	1-5 days[1,4]	Yes[4]		
Diptheria	Contact, droplet inhalation[4]	2-5 days[4]	Yes[4]		
Dysentary	Ingestion, flies, feces[4]	1-7 days[4]	Highly[4]		
Glanders	Horses, mules, asses, droplet inhalation, broken skin[4]	3-5 days[4]	Yes[4]		
Melioidosis (Whitmore's)	Rodent contaminated food, rat fleas[4]	few days[4]	Not typically[4]		
Paratyphoid Fever	Ingestion, infected feces and urine[4]	1-10 days[4]	Yes[4]		
Plague	Insect or animal bites, airborne mucus[1]	1-4 days[1], 1-7days[4]	Yes[1,4]		
Pulmonary Tuberculosis	Inhalation droplets, contact, natural tranmission slow[4]	month[4]	Yes[4]		
Salmonella food poisoning	Ingestion, rodents, food handling (eggs and meat), contact, flies[1,4]	6-48 hours[1,4]	Yes[4]		
Tularemia	Insect or animal bites, inhalation, ingestion, eyes[1,4]	2 -7 days[1], 1-10days[4,5]	No[4]	25[2]	6[5], 30 (inh)[1]
Typhoid Fever	Ingestion, infected feces and urine[1,4]	1-2 wks[1], 3-38days[4]	Yes[4]		
Fungi					
Histoplasmosis	Dust, inhalation (primary), ingestion, broken skin[4]	5-18 days[4]	No[4]		
Nocardiosis	Dust, soil, dry vegetation, inhalation, infection of wounds[4]	Unknown[4]	Possible[4]		
Valley Fever	Dust, soil, dry vegetation, inhalation, skin, ingestion[1,4]	10 to 21 days[4]	No[4]		

Table 2B (continued): Toxicological Properties of Biological Warfare Agents

Common Name	Dissemination/Route of Entry	Incubation/ Onset	Contagious?	50% Infective Dose (organisms/person)	Untreated Lethality (%)
Rickettsia					
Endemic Typhus	Rodent flea bites[4]	6-14 days[4]	No[4]	2[1]	
Epidemic Typhus	Insect bites, inhalation infected louse feces[1,4]	5 - 23 days[1,4]	Yes,lice[4]		
Q fever	Inhalation, ingestion[1,4]	10-28 days[1]	Slight[4]		1[5]
Scrub Typhus	Infected mite bites[4]	1-2 wks[4]	No[4]		
Spotted fever	Insect bites, aerosol inhalation, broken skin[1,4]	2 days-2 wks[1]	No[4]		
Viruses					
Denegue fever	Mosquitos, freeze dried virus[1]	3-6 days[1], 3-15 days[4]	No[4]	Seldom Fatal[1]	
Encephalitis	Insect bites, freeze dried virus[1]	2-15 days[4]	Possible[4]	1[5] (VEE type)	25[5] (VEE type)
Influenza	Mouth and nose excretions, inhalation, contact[1,4]	7-10 days[1], 1-2 days[4]	Highly[4]	variable	
Psittacosis	Infected birds and their excretions[1]	1-4 days[1]		20[1]	
Rift Valley fever	Mosquitos, aerosol excretions, pustulant, freeze dried virus[1]	24-36 hrs[1]			
Smallpox	Person-person, dried scabs, freeze dried virus[1]	7-21 days[4]	Highly[4]		
Yellow fever	Mosquitos, freeze dried virus[1]	1-6 days[1,4]			

Appendix A: Definitions and Units for Airborne Concentrations

Definitions

C = concentration of contaminant = mass concentration of contaminant

= mass fraction of contaminant $\left(\frac{\text{mass of contaminant}}{\text{mass of air - contaminant mixture}}\right)$

$C_{vol} = \frac{M_{air} \bullet C}{M_c + (M_{air} - M_c) \bullet C}$ = volume concentration of contaminant

M_{air} = molecular weight of air = 28.95 amu

M_c = molecular weight of contaminant (e.g., for sarin, = 140.11 amu)

PPM = $10^6 \bullet C_{vol}$ = volume concentration of contaminant in parts per million (ppm)

Note: If $M_c = M_{air}$, then $C_{vol} = C$ and PPM = $10^6 \bullet C$

ρ = density of air - contaminant mixture (mass/volume)

ρ_C = $\rho \bullet C$ = density concentration of contaminant (mass/volume)

Mixture of Contaminant Gas in Air

$\rho = \rho_{air}/[(1 - C) + C \bullet (M_{air}/M_c)]$

ρ_{air} = density of air at 0 °C = 1.29 kg/m^3; at 20 °C = 1.2 kg/m^3

Mixture of Contaminant Particles (Liquid or Solid) in Air

$\rho = \rho_{air}/[(1 - C) + C \bullet (\rho_{air}/\rho_{cp})]$

ρ_{cp} = density of contaminant particles (mass/volume)

Low Concentration Limit

As $C \rightarrow 0$, then $\rho \rightarrow \rho_{air}$ and $\rho_c \rightarrow \rho_{air} \bullet C$

Appendix B Lethal Dose and Exposure Levels for Anthrax and Sarin

Definitions

C = concentration of contaminant $\left(\frac{\text{mass of contaminant}}{\text{mass of air - contaminant mixture}}\right)$

ρ_{air} = density of air (20 °C) = 1.2 kg/m^3 = 1.2 x 10^6 mg/m^3

BR = breathing rate

SR = spore ratio (for biological agents) = spores per mass of contaminant released

Exposure = Time Integrated Concentration = $\int dt \bullet C \bullet \rho_{air}$ (mg-min/m^3)

LCt_{50} = Lethal time-integrated Concentration (Exposure) Level for 50% of the Population (generally use for chemical agents such as sarin)

Dose = $\int dt \bullet C \bullet \rho_{air} \bullet BR \bullet SR$ = Exposure $\bullet$ BR $\bullet$ SR (spores or mass)

LD_{50} = Lethal Dose Level for 50% of the Population (spores or mass) (generally used for biological agents such as anthrax)

Common Units for Comparison of Agents

Converting from Lethal Dose (LD) to Lethal time-integrated Concentration (Exposure) (LCt) gives:

$$LCt\ (\text{mg-min/m}^3) = \frac{LD}{BR \bullet SR}$$

LCt Levels for Sarin

LCt_{50} = 70 (mg-min/m^3) (ref. 7)

Using a probit slope of 12 (ref. 8), the estimated 90% and 10% lethality levels are:

LCt_{90} = 90 (mg-min/m^3)

LCt_{10} = 55 (mg-min/m^3)

LD and LCt Levels for Anthrax

In order to have a common set of units for comparison, we report here values for both the lethal dose (LD) (spores) and the lethal Exposure (LCt) (mg-min/m^3), using a breathing ratio, BR = 0.02 m^3/min (for light activity) (ref. 9), and a spore ratio, SR = 3 x 10^7 spores/mg (ref 10).

LD_{50} = 8,000 spores (ref 5); LCt_{50} = 0.013 (mg-min/m^3)

Based on a probit slope of 0.7 (ref 11), the estimated 90% and 10% lethality levels are:

LD_{90} = 540,000 spores; LCt_{90} = 0.9 (mg-min/m^3)

LD_{10} = 120 spores; LCt_{10} = 0.0002 (mg-min/m^3)

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