

# **Evaluation of the Relative Risk of China Lake 20 (CL-20) Based on Current Toxicity, Fate and Transport, and other Technical Information**

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Ivan Boyer, Ph.D., D.A.B.T.

John K. Miller, M.S.

Rebecca E. Watson, Ph.D.

John DeSesso II, Ph.D., Fellow ATS

Catherine M. Vogel, P.E.

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Falls Church, Virginia

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## Executive Summary

Current toxicity, fate, and transport, and other technical information on China Lake 20 (CL-20) (hexanitrohexaazaisowurtzitane) and other energetic chemicals was summarized, evaluated, and used to conduct a relative risk characterization of CL-20 compared with other chemicals, especially hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX). The toxicology data were determined to be too limited to determine whether CL-20 would likely pose a greater or lesser threat to human health or the environment than RDX or other energetic chemicals in munitions disposal/storage and testing/training areas.

There is no toxicity information for CL-20 in humans or in mammalian, amphibian, and reptilian species. The toxicity data on birds are limited to one species. There are substantially more toxicity data for CL-20 in soil invertebrates and aquatic microorganisms, invertebrates, and animal species. Overall, the data suggest that CL-20 is more toxic than RDX to soil invertebrates. It may also be more toxic than RDX to aquatic animal species. In contrast, CL-20 appears to be less toxic than RDX to birds and plants. However, the limited nature and the uncertainty of this information are too great to allow a comprehensive comparison of the toxicities and potential risks associated with CL-20 and RDX.

The substantial information that has been developed about CL-20 through recent studies has revealed that, generally, the fate and transport of CL-20 is unlikely to differ substantially from that of RDX. Further, limited studies have shown that CL-20, like RDX, has little, if any, propensity to bioconcentrate or bioaccumulate in plants and animals.

CL-20 and RDX differ in two notable respects. First, the environmental degradation of CL-20 can yield glyoxal as an end product, while the breakdown of RDX yields formaldehyde. Glyoxal is formed normally in the body, and the available evidence indicates that, like formaldehyde from RDX, glyoxal from CL-20 would pose little, if any, threat to human health or the environment.

Second, the thermal degradation of CL-20 yields an amorphous solid residue that has not yet been characterized. The threat that this residue may pose to human health or the environment can be assessed only after its constituents are identified and examined for their toxicity, fate, and transport characteristics, and other properties.

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## Acronyms and Abbreviations

<b>ACGIH</b>	American Conference of Governmental Industrial Hygienists
<b>AR</b>	Army Regulation
<b>ATSDR</b>	Agency for Toxic Substances and Disease Registry
<b>BAF</b>	Bioaccumulation factor
<b>BCF</b>	Bioconcentration factor
<b>bw</b>	Body weight
<b>°C</b>	Degree centigrade
<b>CASRN</b>	Chemical Abstracts Service Registry Number
<b>CL-20</b>	China Lake 20; hexanitrohexaazaisowurtzitane
<b>CNS</b>	Central nervous system
<b>CO<sub>2</sub></b>	Carbon dioxide
<b>CSM</b>	Conceptual site model
<b>DA</b>	Department of the Army
<b>DHA</b>	Dehydrogenase activity
<b>DoD</b>	Department of Defense
<b>DWEL</b>	Drinking-Water Equivalent Level
<b>EC<sub>20</sub></b>	20% effective concentration
<b>EC<sub>50</sub></b>	50% effective concentration
<b>EMEG</b>	Environmental Media Evaluation Guide
<b>EPA</b>	Environmental Protection Agency
<b>ESOH</b>	Environmental, safety, and occupational health
<b>Fe<sup>0</sup></b>	Zero valent iron
<b>FETAX</b>	Teratogenesis assay
<b>g</b>	Gram
<b>IC<sub>50</sub></b>	50% inhibitory concentration
<b>HAL</b>	Health Advisory Limit
<b>HBIW</b>	Hexabenzyl hexaazaisowurtzitane
<b>Hg</b>	Mercury
<b>HMX</b>	Cyclotetramethylene-tetranitramine
<b>IC<sub>20</sub></b>	20% Inhibiting Concentration
<b>kg</b>	Kilogram
<b>K<sub>d</sub></b>	Soil-water partition coefficient
<b>K<sub>oc</sub></b>	Solid organic carbon-water partition coefficient
<b>K<sub>ow</sub></b>	Octanol-water partition coefficient
<b>L</b>	Liter
<b>LC<sub>20</sub></b>	20% lethal concentration
<b>LC<sub>50</sub></b>	50% lethal concentration
<b>LD<sub>50</sub></b>	50% lethal dose
<b>LOAEL</b>	Lowest observed adverse effect level
<b>LOEC</b>	Lowest observed effect concentration
<b>m<sup>3</sup></b>	Cubic meter

<b>MC</b>	Munitions constituent
<b>MCL</b>	Maximum Contaminant Level
<b>Me</b>	Methyl
<b>Mg</b>	milligrams
<b>mL</b>	milliliter
<b>mm</b>	millimeter
<b>µg</b>	microgram
<b>µM</b>	micromolar
<b>MIL STD</b>	Military Standard
<b>N<sub>2</sub>O</b>	Nitrous oxide
<b>NA</b>	Not available
<b>NH<sub>3</sub></b>	Ammonia
<b>NOAEL</b>	No observed adverse effect level
<b>NOEC</b>	No observed effect concentration
<b>NOEL</b>	No observed effect level
<b>OB/OD</b>	Open burn/open detonation
<b>OE</b>	Ordnance and explosives
<b>PAH</b>	Polycyclic aromatic hydrocarbons
<b>PNA</b>	Potential nitrification activity
<b>ppb</b>	parts per billion
<b>PRG</b>	Preliminary Remedial Goal
<b>Rac50-50</b>	Composite agricultural-forest soil
<b>RacAg2002</b>	Fine-sandy composite agricultural soil
<b>Racfor2002</b>	Natural sandy forest soil
<b>RBC</b>	Risk-Based Concentration
<b>RDX</b>	hexahydro-1,3,5-trinitro-1,3,5-triazine
<b>R<sub>f</sub>D</b>	Reference dose
<b>SERDP</b>	Strategic Environmental Research and Development Program
<b>SSL</b>	Sassafras Sandy Loam
<b>TADA</b>	Tetraacetyldiamino hexaazaisowurtzitane
<b>TLV</b>	Threshold Limit Value
<b>TNT</b>	2,4,6-trinitrotoluene
<b>UXO</b>	Unexploded ordnance
<b>v/v</b>	volume-to-volume ratio

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# **1 Introduction**

## **1.1 Purpose**

The purpose of this report is to review the current information on China Lake 20 (CL-20) (hexanitrohexaazaisowurtzitane) and other energetic chemicals and to conduct a relative risk characterization of CL-20—to the extent feasible—based on the available information. Specifically, this report attempts to address the question: How do the risks of CL-20 to human health and the environment compare to the risks of other energetic chemicals, especially hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX)?

The Department of Defense's (DoD's) Strategic Environmental Research and Development Program (SERDP) recently funded a substantial research program to determine the physiochemical properties of CL-20 and to characterize its fate and transport properties in the environment and ecotoxicity. This research has produced numerous scientific publications and government technical reports. The present report summarizes and evaluates these studies and similar studies on RDX, cyclotetramethylene tetranitramine (HMX), and 2,4,6-trinitrotoluene (TNT). In addition, this report presents prototypical human and ecological exposure scenarios developed to depict potential exposures to munitions constituents (MCs) that may be associated with disposal/storage and range testing/training activities.

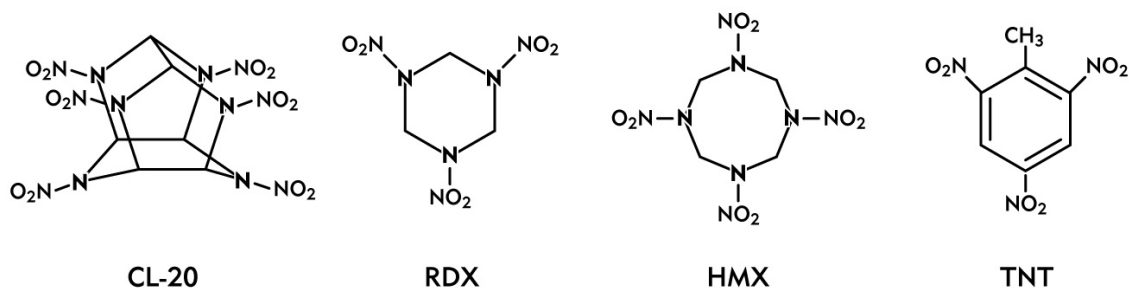
## **1.2 Background**

CL-20 is a new energetic chemical that was first produced in 1987. The advantage of CL-20 is that it has a higher density and delivers more explosive power per pound or unit volume than the other commonly used energetic chemicals. The military has learned over the last decade, however, that the true cost of munitions extends far beyond the production and use of the weapon. Energetic chemicals have caused environmental contamination through use, manufacturing, training, recycling, and demilitarization. In addition, the costs to investigate and remediate these concerns have been increasing. The drive to evaluate new energetic chemicals for their potential impacts to human health and the environment derives from the large sums being spent to investigate and remediate historical energetic chemical manufacturing facilities and training ranges. The military is now aware of potential environmental impacts and of the fact that it must factor these concerns into acquisition programs and estimations of life-cycle costs. Thus, studies of the toxicity and environmental behavior of CL-20 were initiated to help inform the decision to include or not include CL-20 in the military's arsenal.

The basis and authority for these efforts have been incorporated into acquisition-related environmental, safety, and occupational health (ESOH) directives from the DoD and the Services. For example, see DoD Acquisition Directives 5000.1 and 5000.2; Department of the Army (DA) ESOH regulations: DA Pamphlet 70-3, Army Regulation (AR) 70-1, AR 200-1, AR 200-2, AR 40-10, AR 40-5, AR 385-16; and Military Standard (MIL STD) 882. The objectives of the research conducted to characterize the toxicity and the fate and transport of CL-20 before initiating large-scale acquisition of this energetic chemical have included the development of data that can be used to derive ecological benchmarks, which, in turn, can facilitate efforts to estimate the full life-cycle costs of CL-20.

CL-20 has some physical and chemical properties in common with other nitramine explosives, such as RDX and HMX, as well as unique properties. CL-20 is a white powder, a polycyclic

nitramine consisting of multiple rings joined to form a three-dimensional cage structure (Figure 1-1). There are four polymorphic forms of CL-20, referred to as alpha, beta, gamma, and epsilon ( $\alpha$ ,  $\beta$ ,  $\gamma$ , and  $\epsilon$ ). The  $\epsilon$  form is preferred because of its greater density.



**Figure 1-1. Chemical Structure of CL-20, RDX, HMX, and TNT**

In 2001, SERDP began funding research on the toxicity and fate and transport of CL-20, anticipating that CL-20 could be a potential replacement for RDX and other energetic chemicals.

Although the primary objective of this report is to compare the potential environmental and human-health impacts of CL-20 and RDX, information is also provided on HMX and TNT (which is a nitroaromatic explosive). The chemical structure of these substances is depicted in Figure 1-1. TNT and its degradation products are common environmental contaminants in areas where energetic chemicals are manufactured or used. In contrast, HMX rarely drives cleanup efforts because it is less toxic, has less stringent drinking-water advisory levels, and is typically found at relatively low concentrations in groundwater.

### 1.3 Approach

Characterizing the relative risks of CL-20, RDX, and other energetic chemicals was performed by comparatively evaluating information about regulatory requirements and guidelines, exposure scenarios, and parameters of fate, transport, and toxicity.

#### 1.3.1 Regulatory Requirements

Regulatory requirements, standards, and guidelines, along with the pertinent documentation from the regulatory agencies, often represent important sources of readily available information about the hazards, risks, and other relevant issues associated with the release of a compound to the environment. The chemical-specific standards and guidelines developed by these agencies are often based, at least in part, on the results of conservative risk assessments. Although no standards and guidelines currently exist for CL-20, such standards have been developed for related energetic chemicals, such as RDX, HMX, and TNT. The regulatory standards and guidelines for these compounds were evaluated to determine whether they provide insight about standards and guidelines that regulatory agencies might develop for CL-20 in the future. This evaluation is presented in Section 2.

#### 1.3.2 Exposure Scenarios

One of the first steps in the CL-20 evaluation was to develop exposure scenarios or conceptual site models (CSMs). These models were developed to outline and show the potential release, transport, fate, and exposure of humans and other organisms to CL-20 and its degradation

products. In developing these CSMs, CL-20 was assumed to be released during two potential activities:

- Munitions storage, maintenance and disposal operations
- Range testing and training operations

Four CSMs were developed covering these two activities: two for human exposure and two for environmental exposure. Section 3 presents the CSMs, which include potential environmental release mechanisms, pathways, and exposure points.

### **1.3.3 Evaluation Parameters**

The behavior of CL-20 in the environment is largely governed by a set of physicochemical parameters that, together with climatic and hydrogeologic conditions, determine CL-20's fate and transport properties. CL-20 and RDX were compared based on these properties. Section 4.2 addresses the likely fate of these constituents in the environment, and Section 4.3 discusses their environmental transport properties.

The potential for bioconcentration and bioaccumulation of CL-20 and RDX is compared in Section 4.4. Section 4.5 presents a review of the literature on the toxicities of CL-20 and RDX.

### **1.3.4 Relative Risk Evaluation**

The discussion of the relative risk of CL-20 to humans and ecological receptors is presented in Section 5. Unfortunately, this analysis is limited by the paucity of relevant data, which are only beginning to be developed for CL-20. Conclusions and recommendations are presented in Section 6.

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## 2 Regulatory Requirements, Standards, and Guidelines

At this time, there are no human-health or ecological standards for CL-20 because it is a relatively new compound and substantial, widespread, or persistent contamination is unknown. However, the research being performed on the toxicity and environmental degradation of CL-20 could be used to help establish regulatory standards or guidelines for soils and groundwater in the event that CL-20 goes into full-scale production in the future.

This section discusses some of the standards and guidelines available for RDX, HMX, and TNT. This information is presented primarily because CL-20 is chemically related to RDX and HMX in composition, structure, and physicochemical properties. CL-20 also shares with RDX some similar intermediates and many of the same end products of environmental degradation. The similarities of the chemical composition and structure and physicochemical properties of CL-20 with those of RDX and HMX suggest allowable environmental concentrations that could be developed for CL-20 in soils and water in the future. Cleanup concentrations established for RDX and HMX at some facilities, such as Army ammunition plants, are also discussed.

Most human-health standards cover soil and groundwater concentrations and are often scenario-dependent (e.g., industrial/commercial versus residential land-use scenarios). The primary human-health standards for water consumption are the Maximum Contaminant Levels (MCLs), which are legally enforceable drinking-water standards. There are no federal MCLs for the four energetic chemicals reviewed in this report. However, RDX and TNT are included in the U.S. Environmental Protection Agency (EPA) Unregulated Contaminant Monitoring Rule.

Other guidelines developed by the EPA, as well as agencies such as the Agency for Toxic Substances and Disease Registry (ATSDR), are discussed, but it must be emphasized that these values are considered advisory only. Some examples include the EPA's Preliminary Remedial Goals (PRGs), Health Advisory Limits (HALs), and Drinking-Water Equivalent Levels (DWELs), and the ATSDR's Environmental Media Evaluation Guides (EMEGs). MCLs and HALs for lifetime exposure are usually the same.

Protection of aquatic and terrestrial life is also important, and ecological risk screening concentrations are available for surface water and sediment. The ecological risk screening concentrations developed by EPA Region III were considered for this evaluation.

Examples of guidelines for RDX, HMX, and TNT in air, soil, and water are presented in Table 2-1. Note that the air limits listed are time-weighted 8-hour average concentrations designed to address workplace exposures. Regulatory agencies have not developed air limits specifically for the exposure scenarios developed in this evaluation. Further, the low volatility of CL-20, RDX, HMX, and TNT substantially reduces the likelihood that exposure via the air pathway would be significant except, possibly, from the release of these compounds in particulate matter from detonation and low-order explosions.

**Table 2-1. Current Risk-Based Concentrations, Preliminary Remedial Goals, Health Advisory Limits, and Threshold Limit Values for Selected Constituents**

Compound	EPA Region III RBCs/ Region IX PRGs for Soil <sup>1</sup> (mg/kg)		EPA Region III Ecological Risk Values (Chronic)		EPA Water RBCs/PRGs/HALs		ACGIH Air Exposure Guidelines	Water Solubility (20 °C, mg/L) <sup>3</sup>
	Residential (mg/kg)	Industrial (mg/kg)	Water (mg/L)	Sediment (mg/kg)	RBC/PRG <sup>1,2</sup> (mg/L)	HAL (mg/L)	TLV mg/m <sup>3</sup>	
<b>CL-20</b>	NA	NA	NA	NA	NA	NA	NA	3-5
<b>RDX</b>	5.8	26	0.36	0.013	0.00061	0.002	1.5	35-52
	4.4	16			0.00061			
<b>HMX</b>	3,900	51,000	0.15	NA	1.8	0.400	None	5-7
	3,100	31,000			1.8			
<b>TNT</b>	21	95	0.10	0.092	0.0022	0.002	1.5	100
	16	57			0.0022			

1: EPA Region III RBC value (2005) is listed first, followed by Region IX values (2004).

2: Tap water PRGs are generally the same as the federal MCL when a contaminant has an MCL.

3: Solubility data presented in this report are primarily from Monteil-Rivera et al. (2004a) and Lynch (2002).

NA = not available

HAL = EPA Lifetime Health Advisory Limit

TLV = Threshold Limit Value (8-hour time-weighted average) from the American Conference of Government Industrial Hygienists (ACGIH); The TLV for TNT is also the Occupational Safety & Health Administration Permissible Exposure Limit for TNT, which is an enforceable standard.

Although there are no federal cleanup limits for soils, several EPA regional offices have developed risk-based concentrations (RBCs) or PRGs for selected energetic chemicals. The most commonly cited are EPA Region III's RBCs and EPA Region IX's PRGs. In addition, site-specific cleanup goals have been developed for soils at several military sites. These values are generally similar to EPA's soil PRGs for residential scenarios, typically ranging from 2 mg/kg to 60 mg/kg for energetic chemicals such as TNT and RDX, and 3,100 mg/kg for HMX. Cleanup goals for industrial land-use scenarios are generally higher by factors of 4–10.

Except for HMX, the HALs for the energetic chemicals listed in Table 2-1 are more than four orders of magnitude lower than their solubility limits. This illustrates that even though an energetic chemical may have extremely low solubility, it may be sufficient to produce environmental effects. In other words, an energetic chemical's low solubility will not necessarily preclude a threat to human health or the environment.

Site-specific groundwater and soil cleanup goals have been established that are substantially higher than or lower than the guideline values presented in Table 2-1. For example, at the Pantex Plant in Texas, the RDX cleanup goals were set at 0.0077 mg/L for off-site groundwater and 0.026 mg/L for on-site groundwater (Shull et al., 1999). These values are approximately 10 to 40 times higher than the PRG for RDX (0.00061 mg/l). In contrast, at Camp Bonneville, Washington, the soil remediation goals for HMX and RDX—using the state of Washington's Model Toxics Control Act Cleanup Regulations Method B—were set much lower than the soil PRGs (0.5 mg RDX/kg; 3.2 mg HMX/kg [Tetra Tech, 2004]). At the Umatilla Army Depot in Oregon, the cleanup goals for energetic chemicals in soil were set at 30 mg/kg for both RDX and TNT (U.S. EPA, 1997).



These site-specific cleanup goals are similar, but not identical, to the corresponding EPA Region IX industrial PRGs for RDX and TNT.

Generally, the differences between site-specific cleanup goals and the guidelines represented in Table 2-1 are attributable to differences in the nature and basis of site-specific goals and the guideline values. RBCs, PRGs, and ecological screening values are typically derived based on highly conservative, generic exposure assumptions and are meant to be used in preliminary or screening-level assessments of a site or an area. They cannot usually serve as a credible or technically defensible basis for deciding to remediate a site or as final remediation goals for the site. In contrast, final remediation goals are ordinarily developed based on a site-specific assessment of exposure scenarios, pathways, receptors, and other data available for the site.

Finally, it is important to note that soil RBCs and PRGs, such as those presented in Table 2-1, are developed to address the soil ingestion route of exposure. Thus, these values are generally not considered protective of groundwater resources that might be contaminated through the migration of constituents from soil to groundwater. Methods for estimating soil cleanup levels for the protection of groundwater resources have typically yielded soil cleanup goals about two orders of magnitude *lower* than the soil RBCs and PRGs. For example, if the HAL for RDX (0.002 mg/L) is used to derive a soil cleanup goal where a soil contaminant may migrate to groundwater, the cleanup goal for soil would be 0.2 mg/kg, which is 100 times the HAL and about 1/20<sup>th</sup> of the soil RBC.

There is no information available to estimate the potential toxicity of CL-20 to human health. If the development of such data indicates toxicity similar to that of RDX, then future standards and guidelines that might be developed for CL-20 may be similar to those for RDX, as presented in Table 2-1. Further, if the controlling factor for soil cleanup of CL-20 was the protection of groundwater resources, then, like RDX, the soil cleanup goal might be less than 1 mg/kg. However, these observations remain highly speculative without adequate toxicity data for CL-20.

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### 3 Exposure Scenarios

Several human and ecological exposure scenarios were developed to depict the potential exposures to CL-20 and RDX considered in this evaluation. Although some of the largest and most concentrated environmental releases of energetic chemicals have historically occurred during weapons manufacturing and demilitarization, these types of releases are not within the scope of this evaluation, partly because modern manufacturing and demilitarization practices are anticipated to substantially limit the contamination expected from these activities when compared with past practices. The chosen scenarios were categorized and consolidated to develop four generic CSMs depicted in Figures 3-1 through 3-4. The CSMs display the interrelationships among the major sources of contamination, potential release mechanisms, migration pathways (including media that may become secondary and tertiary sources), exposure locations and exposure media, and human and ecological receptors potentially affected by exposures to MCs in the environment. MCs include the explosive (e.g., CL-20, RDX, HMX and TNT) and non-explosive chemicals in munitions, as well as the breakdown products of these chemicals (e.g., products of combustion, detonation, and hydrolysis).

Figures 3-1 through 3-4 depict the CSMs for two hypothetical sites, each representing a major category of munitions-related activities. The assumed activities include munitions storage and disposal at one site (Figures 3-1 and 3-2) and munitions testing and training at another site (Figures 3-3 and 3-4). Two CSMs are presented for each site, including one for human receptors (Figures 3-1 and 3-3) and another for ecological receptors (Figures 3-2 and 3-4). The CSMs and the exposure scenarios that they represent are discussed in greater detail below.

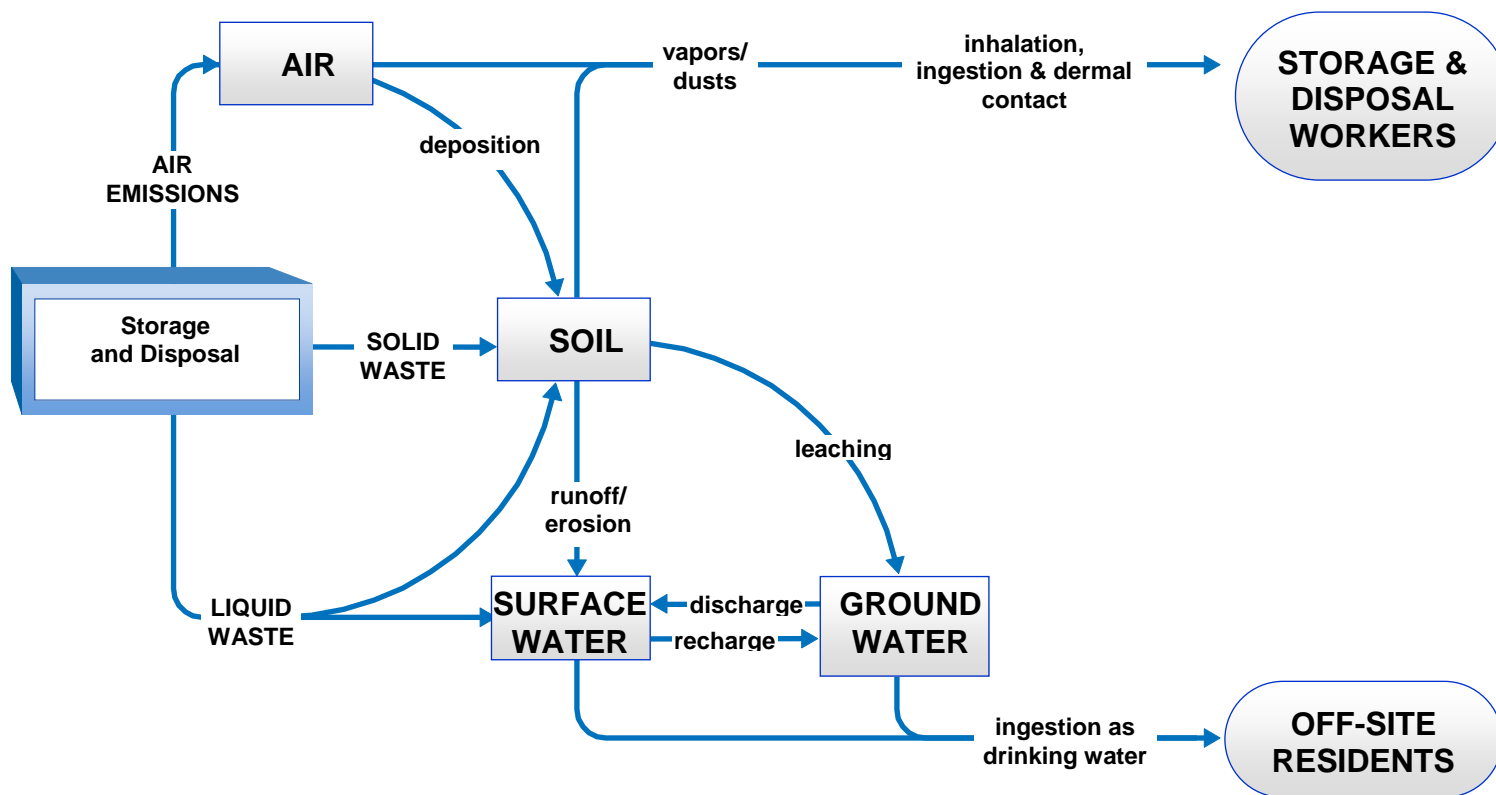
#### 3.1 Storage and Disposal Site

Figures 3-1 and 3-2 illustrate the potential exposure of humans and ecological receptors, respectively, to MCs at a storage and disposal site. Ordnance-related activities at this site may include, for example, storage in ammunition piers and ordnance magazines, handling at ammunition transfer points, and disposal by open burn/open detonation (OB/OD) or non-thermal methods (e.g., chemical neutralization).

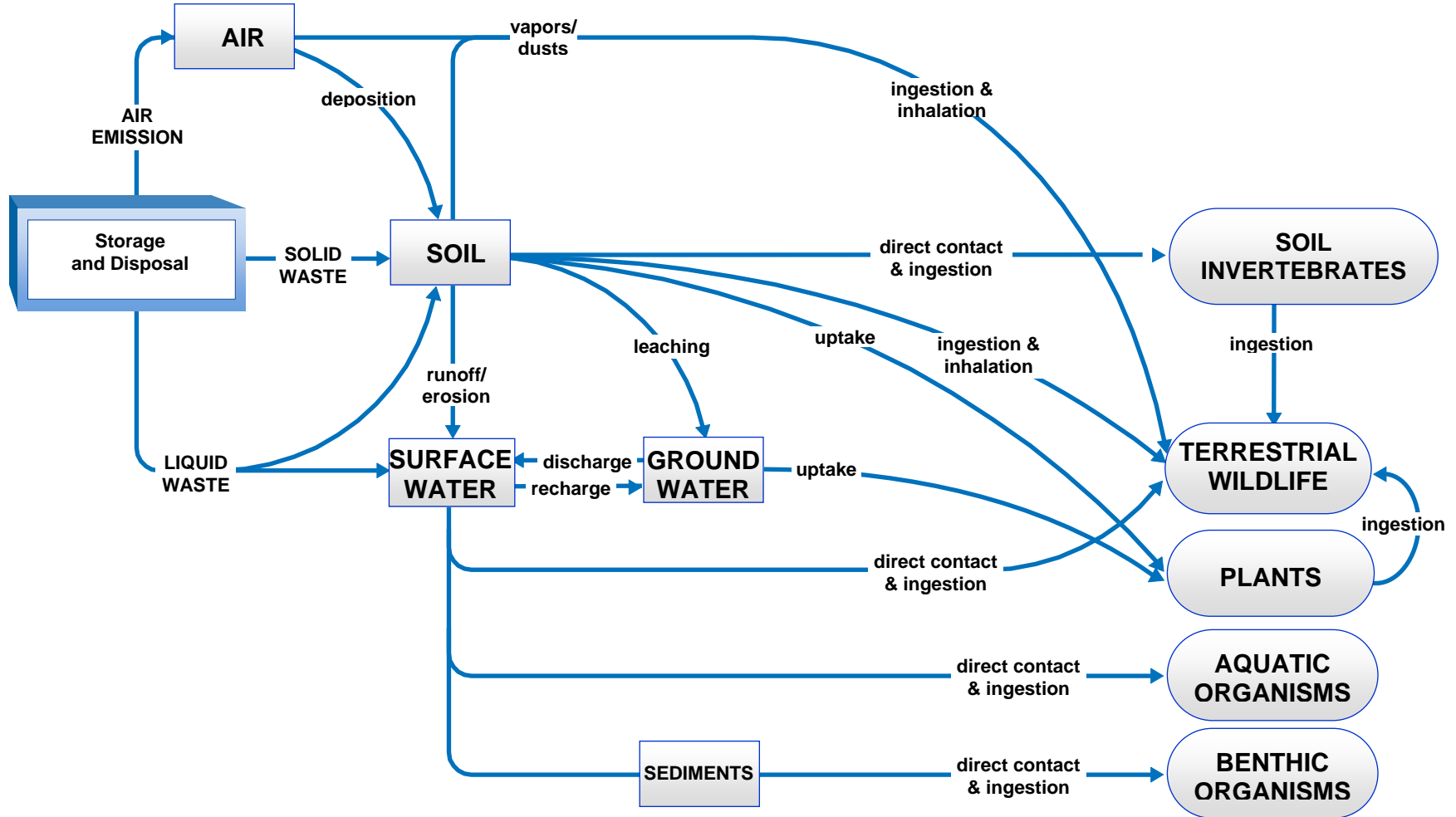
##### 3.1.1 Sources of Contamination

The primary mechanisms assumed for the release of MCs to the environment at the storage and disposal site include mishandling, loss, and abandonment of munitions in storage or transfer areas; “kick-outs” (e.g., ejection of residues from blow-in-place procedures to destroy unexploded ordnance [UXO]) and low-order detonations in OB/OD areas; and deposition of liquid wastes from non-thermal disposal methods (e.g., base hydrolysis). These release mechanisms can be expected to contaminate air, soil, and surface water with MCs.

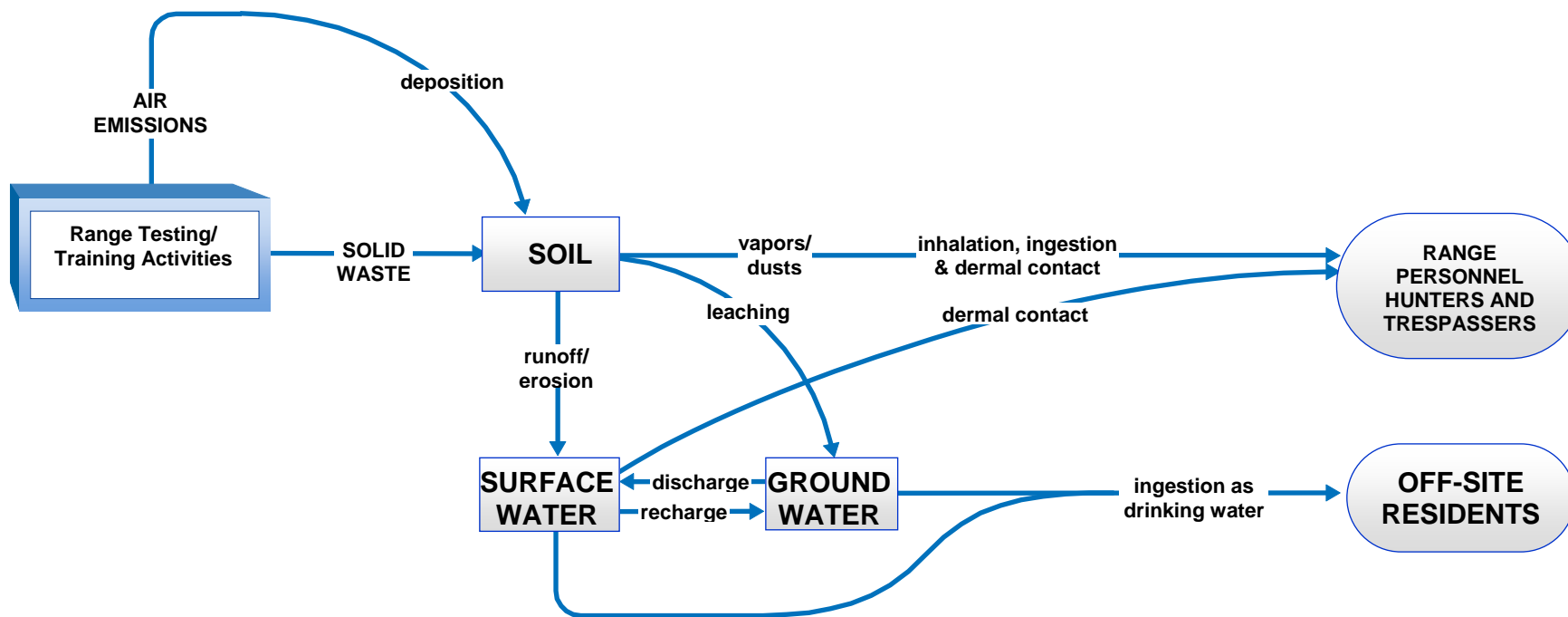
For example, kick-outs from OB/OD disposal will disperse MCs directly into the overlying air and the underlying soil, and scatter ordnance components and debris over the surrounding surface soil and into the underlying soil. Some of the MCs may be released to the air as vapors and fine dusts that dissipate with increasing distance from the site. Others may be released to the air as chunks, particles, and dusts that settle on nearby surface soil and in surface water. In addition, MCs associated with ordnance components and debris may be leached to the soil surface or emitted to the air over time. Other munitions disposal methods, such as base hydrolysis, may result in the release of MCs in liquid wastes directly to soil and surface water.



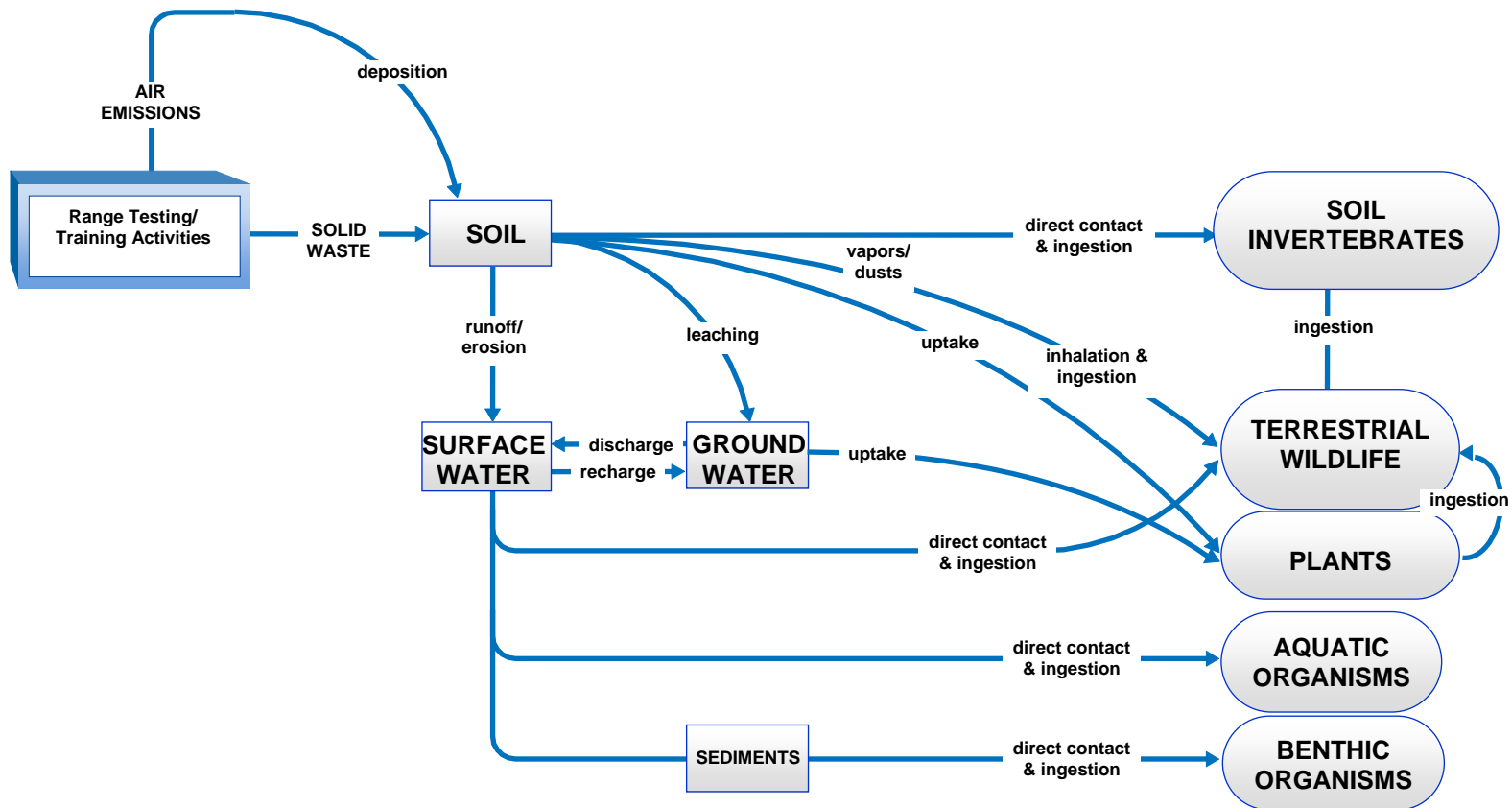
**Figure 3-1. Conceptual Site Model: Potential Human Exposure to Munitions Constituents from Disposal and Storage Activities**



**Figure 3-2. Conceptual Site Model: Potential Ecological-Receptor Exposure to Munitions Constituents from Disposal and Storage Activities**



**Figure 3-3. Conceptual Site Model: Potential Human Exposure to Munitions Constituents from Range Testing/Training Activities**



**Figure 3-4. Conceptual Site Model: Potential Ecological-Receptor Exposure to Munitions Constituents from Range Testing/Training Activities**

### **3.1.2 Transport Pathways**

The primary media assumed to be contaminated at the storage and disposal site are air, soil, and surface water, as discussed in Section 3.1.1 and illustrated in Figures 3-1 and 3-2.

Secondary release mechanisms assumed for this site include deposition of MCs in air to the surface soil; migration of MCs from soil to air, surface water, and groundwater; and migration of MCs in surface water to groundwater. Constituents in surface soil can enter air as vapors, powders, or dusts, depending on their volatility, purity, and affinity for the soil and on the environmental conditions, including the characteristics of the soil (e.g., moisture and fine particulate content), the climate (e.g., temperature, wind speed, precipitation), and other site-specific factors. Constituents in the surface soil may also leach into groundwater or enter surface water through rain run-off and erosion.

Surface water and groundwater may also be contaminated by tertiary release mechanisms. For example, a creek contaminated through the erosion of soil at the site may recharge groundwater located downstream of the point where the contaminated soil enters the creek. Similarly, groundwater contaminated through leaching from the surface soil at the site may discharge to a surface water body located downgradient of the site. These mechanisms will depend on site-specific hydrological characteristics.

### **3.1.3 Potential Human Receptors**

As indicated in Figure 3-1, human receptors assumed for the storage and disposal site include on-site storage and disposal workers, and off-site residents.

Storage and disposal workers include personnel that handle, transfer, or transport ordnance and explosives (OE), and conduct, support, or manage operations or maintenance in a storage facility or disposal area. These workers may be exposed to MCs in the air and soil at the site through inhalation, ingestion, or dermal contact.

Off-site residents are found in areas where people are housed, educated, or cared for (e.g., day-care centers, schools, medical facilities, and nursing homes), including on-base family and non-family housing areas and off-base residential areas. The most likely residential receptors are located downgradient or downstream of the site, where they may be exposed to MCs in groundwater or surface water used as drinking water and for other household purposes (e.g., bathing, showering, cooking, and washing clothes and dishes).

The ingestion of water used by off-site residents as drinking water represents exposures to MCs in water by all potential routes for these receptors, including the following:

- Inhalation and ingestion of MCs in water used for cooking
- Inhalation of and dermal contact with MCs in water used for bathing and showering
- Ingestion of MCs in homegrown produce that is irrigated with contaminated water
- Incidental ingestion and dermal contact with MCs in surface water while swimming or wading

In addition, potential inhalation exposures to MCs in the air are assumed to be negligible even for residents located predominantly downwind of the site. This is because MCs released to the air at the site are assumed to dissipate or settle out before reaching residential areas.



### **3.1.4 Potential Ecological Receptors**

As illustrated in Figure 3-2, ecological receptors assumed for the storage and disposal site include on-site soil invertebrates, plants, aquatic and benthic organisms, and terrestrial wildlife. Soil invertebrates (e.g., earthworms and terrestrial insects), aquatic organisms (e.g., fish, amphibians, and aquatic insects), and benthic organisms (e.g. crustaceans and benthic microorganisms) may be exposed to MCs by ingestion or by direct contact with MCs in soil, surface water, and sediment, respectively. Plants (e.g., grasses, forbs, shrubs, and trees) may be exposed to MCs in soil and groundwater through root uptake. Terrestrial wildlife (e.g., burrowing and non-burrowing birds, reptiles, and mammals) may be exposed to MCs in air, soil, and surface water by inhalation and ingestion and in the food chain by consumption of prey (e.g., earthworms, insects) or plants (e.g., fruits, seeds, leaves).

For the purpose of this assessment, dermal contact with MCs in air and soil is considered negligible for wildlife when compared with exposures through ingestion and inhalation, because fur, feathers, and scales represent a barrier to skin contact. Particulate matter that adheres to fur, feathers, or scales can be expected to enter the body primarily through ingestion during preening, grooming, or cleaning activities. In addition, the incidental ingestion of MCs in sediments by dabbling fowl in shallow water bodies and the foliar uptake by plants of MCs in air and surface water is assumed to be negligible.

## **3.2 Testing and Training Site**

Figures 3-3 and 3-4 illustrate the potential exposure of humans and ecological receptors, respectively, to MCs at a test and training range. Ordnance-related activities at this site may include, for example, munitions or explosives/propellants testing on a test range or in a test facility, weapons training at firing points or in aircraft, or troop training in a maneuver or bivouac area.

### **3.2.1 Sources of Contamination**

The primary mechanisms assumed for the release of MCs to the environment at the test and training range include mishandling, loss, abandonment, and burial of munitions at firing points; high-order and low-order detonations; and spent munitions and duds in impact areas, on bombing targets, or within range safety fans. These release mechanisms can be expected to contaminate air and soil with MCs.

For example, aerial bombing of a target will disperse MCs directly into the overlying air and the underlying soil, and scatter ordnance components and debris over the surrounding surface soil and into the underlying soil. Some of the MCs may be released to the air as vapors and fine dusts that dissipate with increasing distance from the site. Others may be released to the air as chunks, particles, and dusts that settle on nearby surface soil.

### **3.2.2 Transport Pathways**

The primary media assumed to be contaminated at the test and training range are soil and surface water, as discussed in Section 3.2.1 and illustrated in Figures 3-3 and 3-4.

Secondary release mechanisms assumed for this site include the migration of MCs from soil to air, surface water and groundwater; and the migration of MCs from surface water to groundwater.

As for the storage and disposal site (see Section 3.1.2), constituents in surface soil at the test and training range can enter air as vapors, powders, or dusts; leach into groundwater; or enter surface water through run-off and erosion. In addition, surface water and groundwater may be contaminated by tertiary release mechanisms.

### **3.2.3 Potential Human Receptors**

As depicted in Figure 3-3, human receptors for the test and training range may include on-site range personnel, recreational hunters, trespassers, and off-site residents.

Range personnel include workers that periodically conduct, support, or manage testing and training operations or maintenance of the range. Hunters may be allowed at times in the range area, and trespassers may be assumed to have a presence in areas of the range containing attractive features (e.g., fields, woods, or surface-water bodies). Range personnel, hunters, and trespassers may be exposed to MCs in the soil/dust at the site through inhalation, ingestion, and dermal contact and in surface water through dermal contact while wading.

Ingestion of MCs in wild game taken by hunters; incidental ingestion of surface water by trespassers while swimming; and inhalation of airborne emissions by range personnel, hunters and trespassers during test and training exercises are assumed to be negligible.

Off-site residents are found in areas where people are housed, educated, or cared for, as described in Section 3.1.3 for the storage and disposal site. The ingestion of water used by off-site residents as drinking water represents exposures to MCs in water by all potential routes, as detailed in Section 3.1.3. In addition, potential inhalation exposures to MCs in the air are assumed to be negligible.

### **3.2.4 Potential Ecological Receptors**

As indicated in Figure 3-4, ecological receptors assumed for the test and training range include on-site soil invertebrates, plants, aquatic and benthic organisms, and terrestrial wildlife. Dermal contact with MCs in soil and incidental ingestion of MCs in sediments are considered negligible for wildlife, and foliar uptake of MCs in air is considered negligible for plants, as discussed in Section 3.1.4 for the storage and disposal site. Inhalation of airborne emissions during test and training exercises on the range is also assumed to be negligible for wildlife.

## 4 Comparison of Evaluation Parameters

### 4.1 Physicochemical Properties of CL-20, RDX, TNT, and HMX

Although this report primarily compares CL-20 and RDX, the physicochemical properties of HMX and TNT are included because these two compounds are also common energetic chemicals, and CL-20 could possibly be used as a replacement for them.

All of these energetic chemicals contain the same elements—carbon, nitrogen, hydrogen, and oxygen—arranged in ring complexes. In the case of CL-20, there are two joined ring complexes. CL-20 has the highest molecular weight and most complicated chemical structure of all of these compounds. The high density of CL-20 explains, in part, the higher explosive energy per pound of CL-20 relative to the other explosives listed in Table 4-1. Bhushan et al. (2004b) noted that the structural similarities among CL-20, RDX, and HMX suggest that CL-20, if used in a manner similar to RDX, may yield similar environmental concerns in soil, sediment, and groundwater.

Each physicochemical property listed in Table 4-1 is discussed individually. However, each compound's relative impact on human health and the environment will depend collectively on its physiochemical properties, how the compound is introduced into the environment, and the environmental conditions at release points and along migration pathways.

**Table 4-1. Basic Physicochemical Properties of CL-20, RDX, TNT, and HMX**

Compound	Molecular Weight	Density (20°C)	Water Solubility (mg/L at 5, 20, & 40°C)	Soil Sorption $K_d$	Log $K_{oc}$	Vapor Pressure Torr (mm Hg)
CL-20	438	2.04	2, 3-5, 7.4	0.22-3.8	2.4-3.2	ND
RDX	222	1.82	16, 35-52, 123	0.16-3.5	0.89-2.4	$4 \times 10^{-9}$
HMX	296	1.91	1.3, 3-7, 11.8	0.086-18	0.54-2.8	$3 \times 10^{-14}$
TNT	227	1.65	57, 100, 245	0.04-11	2.5-3.0	$2 \times 10^{-4}$

Densities are from Hoffman (2003), the Merck Index and ATSDR (1997); Density is for the pure  $\epsilon$  form of CL-20, and will vary by formulation. Solubility data are primarily from Monteil-Rivera et al. (2004a) and Lynch (2002). The  $K_d$  values are from Brannon et al. (1999) and Szecsody et al. (2004).  $K_{oc}$  values are from ATSDR (1995b, 1997), Townsend and Myers (1996) and Hawari et al. (2003). Vapor pressures are from HSDB and Rosenblatt et al. (1991). ND = not determined

#### 4.1.1 Aqueous Solubility

Solubility is one of the factors that controls the mobility and persistence of a compound in soils at the point of release to the environment. All other factors being equal, a compound with lower solubility is generally likely to remain in soils longer than a compound with higher solubility. In addition, the upper limit of concentrations that one might expect in groundwater or surface water cannot exceed the solubility limit of the compound. Concentrations in groundwater and surface water are typically only a few percent or less of the compound's solubility limit because of dilution, dispersion, and degradation.

On an absolute scale, the four energetic chemicals evaluated have very low aqueous solubilities and are considered essentially insoluble. However, as will be discussed later, even very low concentrations of these compounds in water may have a potential effect on human health or the environment.

CL-20 generally has the lowest solubility of the four compounds listed in Table 4-1. Its solubility is  $1/8^{\text{th}}$  to about  $1/17^{\text{th}}$  of that of RDX and about  $1/30^{\text{th}}$  of that of TNT. The solubility of HMX at  $20^{\circ}\text{C}$  is slightly greater than that of CL-20. Although solubility generally increases with temperature, CL-20 shows the lowest rate of increase with temperature of the energetic chemicals listed in Table 4-1. For example, over the temperature range of  $5^{\circ}\text{C}$  to  $40^{\circ}\text{C}$ , the solubility of RDX increases by a factor of 7.7, while that of CL-20 increases only by a factor of 3.7. Thus, considering only solubility, CL-20 could be expected to remain in soil at the release point much longer than RDX in tropical environments. Furthermore, the concentrations of RDX compared to those of CL-20 could be substantially greater in warmer tropical groundwater because of RDX's much greater solubility under these conditions.

In a study by Kuperman et al. (2006a), CL-20 concentrations in soil leachates never reached the solubility limit of about 5 mg/L but slowly increased over 11 weeks, becoming relatively stable at approximately 0.5 and 2 mg/L in soils containing 98.4 mg/kg and 9,555 mg/kg of CL-20, respectively. Thus, the stable concentrations in the leachates represented 0.5 percent and 0.02 percent of the concentrations of CL-20 in the soil samples. These results suggest a reasonably high potential for slow leaching and long-term transport of CL-20 to groundwater, as well as indicate that groundwater concentrations will likely be well below the solubility limit of CL-20.

As expected, the dissolution rate of TNT is the highest of the four compounds. HMX dissolves faster than RDX even though the solubility of RDX is higher than HMX at the same temperature (Lynch, 2002). Characteristically, the dissolution rates of energetic chemicals in the chemical mixtures used in munitions are lower than the dissolution rates of the unmixed chemicals. The energetic chemicals are generally mixed with other materials to bind or enhance certain properties. The dissolution rates relative to the unmixed energetic chemicals are typically lower by factors of 2 to greater than 10 compared with those of the corresponding unmixed energetic chemical, depending on the formulation. Further, energetic chemicals contained in whole or in part within the casing of a munition, such as in UXO on a range, can be expected to remain in place much longer than constituents that are not contained in this manner.

In addition, the relatively low solubility of CL-20 indicates that groundwater plumes will have slightly lower concentrations and slightly smaller dimensions than those of RDX under similar conditions and release concentrations. However, tests conducted by the Cold Regions Research and Engineering Laboratory indicated that, once dissolved in water, CL-20 will probably behave similarly to RDX and HMX (Jenkins et al., 2003).

#### **4.1.2 Soil-Water Partition Coefficient ( $K_d$ )**

The *soil-water partition coefficient* ( $K_d$ ) is a mathematical expression that describes the equilibrium distribution of a chemical compound between soil and water. Sorption is the process whereby a dissolved substance becomes attached to a solid particle in the soil or aquifer matrix, typically organic matter, clays, or oxides of iron and manganese. When a compound is sorbed, it is removed from solution and held by the solid material. In groundwater, sorption is defined as the attraction of a dissolved species (e.g., CL-20 or RDX) to the solid materials in the aquifer (the geologic materials). The sorption in groundwater depends on the characteristics of the dissolved species and the aquifer materials. Substances that are highly sorbed tend to move more slowly than the groundwater, while substances that are only slightly or poorly sorbed move at nearly the same rate as groundwater.

Therefore, sorption must be taken into consideration when estimating contaminant transport times and distances.

Sorption removes the compound from solution until the ability of the material to sorb the compound or the compound itself is exhausted. This process affects the mobility, degradation, and toxicity of the compound by reducing its availability. A fundamental understanding of sorption and desorption mechanisms is essential for assessing the fate and impact of a compound in soils and groundwater. Factors affecting sorption include the chemical characteristics of the inorganic and organic fractions of the medium, chemical characteristics of the solute, temperature, and pH.

A contaminant is more likely to be sorbed when the dissolved contaminant passes through soil or aquifer materials that contain significant amounts of one or more of the following:

- Organic matter
- Silt and clay minerals
- Oxides of manganese and iron

The relative importance of each of these aquifer materials varies by compound and may not be important in all cases. Materials such as clean sands without organic matter, iron and manganese oxides, or clays tend to have low sorption capacities (low  $K_d$ ), and any of the dissolved energetic chemicals will tend to move at the same rate as the water. Aquifer materials containing clays, organic matter, or iron/manganese oxides will tend to sorb and retard some energetic chemicals, which means that their rate of movement would be somewhat less than the groundwater.

Because there is very little difference in the  $K_{ds}$  for CL-20 and RDX, both compounds might be viewed as likely to exhibit the same degree of sorption—which is low. However, it is important to note that sorption will be highly dependent on the type of sorbent. For example, RDX and HMX sorption have been shown to be correlated to clay content, while CL-20 is correlated to organic matter (Balakrishnan et al., 2004b; Szecsody et al., 2005). Thus, even though CL-20 and RDX may have similar  $K_{ds}$ , there can still be differences in their behavior based on the type of soil or aquifer materials.

Relatively high  $K_{ds}$  (up to ~300) were reported for CL-20 in soils with high organic content, depending on the type—as well as the amount—of organic matter in the soils (Balakrishnan, et al., 2004b; Hawari et al., 2003). Thus, there may be some noteworthy differences in the movement of CL-20 and RDX through matrices with large amounts of certain, as yet undefined, types of organic matter and little clay content (and vice versa).

However, the physicochemical measurements reported by Monteil-Rivera et al. (2004a), for example, indicate that both CL-20 and RDX can generally be expected to be poorly immobilized in soil, sediment, and groundwater matrices. Thus, if CL-20 were used in the same manner and to the same extent as RDX, groundwater plumes would likely result and present environmental concerns similar to those reported for RDX.

#### **4.1.3 Vapor Pressure or Volatilization**

Energetic chemicals are typically solid compounds, and their volatilization is usually viewed as insufficient to provide an exposure pathway. The vapor pressures of RDX, HMX, and TNT at 20°C are quite low ( $\sim 10^{-5}$  to  $10^{-14}$  Torr [mm Hg]). In comparison, water has a vapor pressure of about 17.5 at 20°C, which is more than 1 million times greater than that of RDX. Although no data on

vapor pressure were found for CL-20, it is expected to have a vapor pressure in the same range as RDX, and volatilization of CL-20 is expected to be similar to RDX. Thus, neither CL-20 nor RDX should have a significant volatilization potential under normal environmental conditions.

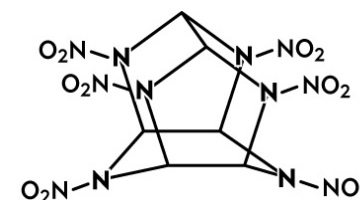
## **4.2 Environmental Fate of CL-20, RDX, and TNT**

Substantial research has been conducted on the degradation of CL-20 by environmental agents, including microorganisms and enzymes derived from microorganisms, light, iron ( $Fe^0$ ), and alkaline soil and water. The degradation end products produced by these diverse agents are remarkably similar (Table 4-2), indicating that CL-20 will yield a characteristic set of end products in the environment regardless of environmental conditions and breakdown mechanisms. Some of the intermediate degradation products of CL-20 have complex ring structures, including highly strained structures, and are characterized by multiple nitro groups ( $-NO_2$ ). The characteristics of these intermediates indicate that, like CL-20 itself, they will be generally unstable and will readily mineralize in the environment.

Other CL-20 breakdown products will be similarly labile. For example, nitramide ( $NH_2NO_2$ ) will rapidly break down to form ammonia ( $NH_3$ ) and nitrous oxide ( $N_2O$ ) in water or in moist soil (Bhushan et al., 2005). Thus, the end products of CL-20 degradation may include ammonia, carbon dioxide ( $CO_2$ ), formate, glyoxal, nitrate and nitrite, nitrogen, and nitrous oxide. Gases—such as  $CO_2$ , nitrogen, and nitrous oxide—would be expected to dissolve to some extent in water, including soil pore water, but they would primarily be released to the atmosphere. Nitrous oxide would rapidly dissipate in the air, so that hazardous air concentrations are improbable and would pose no threat to human health or the environment. Other products, such as formate and glyoxal, will mineralize, and nitrate will yield nitrite to an extent and at a rate that will depend on environmental conditions.

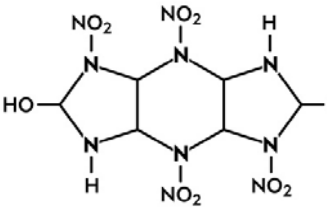
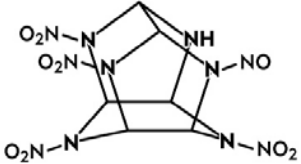
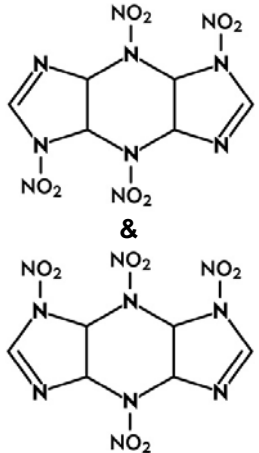
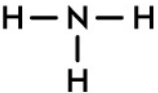

Studies on the breakdown of RDX reveal that an array of breakdown end products can be expected in the environment remarkably similar to those of CL-20 (Table 4-3). Many of the intermediates are nitrated ring structures or ring cleavage products that are not expected to persist in the environment. Generally, these products will be rapidly degraded further to form additional labile intermediates (e.g., nitramide and formamide, which break down rapidly in water to form ammonia and formaldehyde) or simply mineralize. As for CL-20, the end products of RDX degradation may include ammonia,  $CO_2$ , formate, nitrate and nitrite, and nitrous oxide; however, the breakdown of RDX yields formaldehyde rather than the glyoxal produced from CL-20 degradation.

**Table 4-2. Environmental Degradation Products of CL-20**



CASRN	Degradation Product (Chemical Formula)	Agent (Conditions)	Reference	Chemical Structure
830321-13-6	C <sub>6</sub> H <sub>6</sub> N <sub>12</sub> O <sub>11</sub> (Mononitroso Derivative of CL-20)	<i>Clostridium sp. EDB2</i> , Isolated and Purified Enzyme	Bhushan et al., 2005	<p>The structure shows a 1,3,5-triazine ring with nitro groups at the 2, 4, and 6 positions, and a mononitroso group (-NO) at the 1 position.</p>
		<i>Clostridium sp. EDB2</i> , Marine Isolate (Anaerobic)	Bhushan et al., 2004c	
		Zero Valent Iron (Fe <sup>0</sup> ) (Anaerobic)	Balakrishnan et al, 2004a	
None	C <sub>6</sub> H <sub>7</sub> N <sub>11</sub> O <sub>11</sub>	Photolysis	Hawari et al., 2004	<p>The structure shows two possible photolysis products: a 1,3,5-triazine ring with nitro groups at the 2, 4, and 6 positions, and a hydroxyl group (-OH) at the 1 position; and a 1,3,5-triazine ring with nitro groups at the 2, 4, and 6 positions, and a carbonyl group (=O) at the 1 position.</p>
None	C <sub>6</sub> H <sub>6</sub> N <sub>12</sub> O <sub>10</sub> (Dinitroso Derivative of CL-20)	Zero Valent Iron (Fe <sup>0</sup> ) (Anaerobic)	Balakrishnan et al, 2004a	<p>The structure shows a 1,3,5-triazine ring with nitro groups at the 2, 4, and 6 positions, and dinitroso groups (-NO) at the 1 and 3 positions.</p>
289042-67-7	C <sub>6</sub> H <sub>7</sub> N <sub>11</sub> O <sub>10</sub> (Dinitrohydrogenated CL-20)	<i>Clostridium sp. EDB2</i> , Isolated and Purified Enzyme	Bhushan et al., 2005	<p>The structure shows a 1,3,5-triazine ring with nitro groups at the 2, 4, and 6 positions, and a hydrogen atom (-H) at the 1 position.</p>
		<i>Clostridium sp. EDB2</i> , Marine Isolate (Anaerobic)	Bhushan et al., 2004c	
		Zero Valent Iron (Fe <sup>0</sup> ) (Anaerobic)	Balakrishnan et al, 2004a	

**Table 4-2. Environmental Degradation Products of CL-20 (Continued)**

CASRN	Degradation Product (Chemical Formula)	Agent (Conditions)	Reference	Chemical Structure
None	C <sub>6</sub> H <sub>10</sub> N <sub>10</sub> O <sub>10</sub> (Carbinol Adduct; α-Hydroxyalkyl Nitramine)	Nitroreductase from <i>Escherichia coli</i>	Bhushan et al., 2004a	
		Salicylate 1-Monooxygenase from <i>Pseudomonas sp. ATCC 29352</i>	Bhushan et al. 2004b	
		Zero Valent Iron (Fe <sup>0</sup> ) (Anaerobic)	Balakrishnan et al, 2004a	
None	C <sub>6</sub> H <sub>7</sub> N <sub>11</sub> O <sub>9</sub> (Dinitrohydrogenated Mononitroso CL-20)	Zero Valent Iron (Fe <sup>0</sup> ) (Anaerobic)	Balakrishnan et al, 2004a	
763128-26-3 & 763128-28-5	C <sub>6</sub> H <sub>6</sub> N <sub>10</sub> O <sub>8</sub> (Doubly Denitrated CL-20)	<i>Clostridium sp. EDB2</i> , Isolated and Purified Enzyme	Bhushan et al., 2005	
		<i>Clostridium sp. EDB2</i> , Marine Isolate (Anaerobic)	Bhushan et al., 2004c	
		Manganese peroxidase (MnP)	Fournier et al., 2006	
		Nitroreductase from <i>Escherichia coli</i>	Bhushan et al., 2004a	
		Photolysis	Hawari et al., 2004	
		Salicylate 1-Monooxygenase from <i>Pseudomonas sp. Strain ATCC29352</i>	Bhushan et al. 2004b	
		Zero Valent Iron (Fe <sup>0</sup> ) (Anaerobic)	Balakrishnan et al, 2004a	
7664-41-7	Ammonia (NH <sub>3</sub> )	Alkaline Hydrolysis (pH 10)	Balakrishnan et al., 2003	
		Nitroreductase from <i>Escherichia coli</i>	Bhushan et al., 2004a	
		Photolysis	Hawari et al., 2004	
		Salicylate 1-Monooxygenase from <i>Pseudomonas sp. Strain ATCC29352</i>	Bhushan et al. 2004b	
		Soil	Kuperman et al., 2006b	
		Zero Valent Iron (Fe <sup>0</sup> ) (Anaerobic)	Balakrishnan et al, 2004a	
124-38-9	Carbon Dioxide (CO <sub>2</sub> )	<i>Irpex lacteus</i> (Aerobic)	Fournier et al., 2006	
		<i>Phanerochaete chrysosporium</i> (Aerobic)	Fournier et al., 2006	



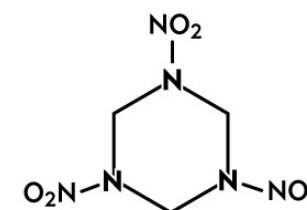
**Table 4-2. Environmental Degradation Products of CL-20 (Continued)**

CASRN	Degradation Product (Chemical Formula)	Agent (Conditions)	Reference	Chemical Structure
64-18-6	Formic acid (CH <sub>2</sub> O <sub>2</sub> )	Alkaline Hydrolysis (pH 10)	Balakrishnan et al., 2003	$\text{O}=\text{CH}-\text{OH}$
		Alkaline Hydrolysis (pH 9.5)	Szecsody et al., 2004	
		<i>Clostridium sp. EDB2</i> , Isolated and Purified Enzyme	Bhushan et al., 2005	
		<i>Clostridium sp. EDB2</i> , Marine Isolate (Anaerobic)	Bhushan et al., 2004c	
		Glass, Aqueous (Oxic)	Monteil-Rivera et al., 2004a	
		Hectorite	Szecsody et al., 2004	
		Nitroreductase from <i>Escherichia coli</i>	Bhushan et al., 2004a	
		Photolysis	Hawari et al., 2004	
		<i>Pseudomonas sp.</i> Strain FA1, Membrane-Enzyme Preparation	Bhushan et al., 2003a	
		Salicylate 1-Monooxygenase from <i>Pseudomonas sp.</i> Strain ATCC29352	Bhushan et al. 2004b	
		Soil (Weathering & Aging)	Kuperman et al., 2006b	
		Subsurface Sediment, Burbank (Oxic)	Szecsody et al., 2004	
		Subsurface Sediment, Norborne (Oxic)	Szecsody et al., 2004	
		Subsurface Sediment, Norborne (Reduced)	Szecsody et al., 2004	
		Subsurface Sediment, Ocala (Oxic)	Szecsody et al., 2004	
107-22-2	Glyoxal (C <sub>2</sub> H <sub>2</sub> O <sub>2</sub> )	Zero Valent Iron (Fe <sup>0</sup> ) (Anaerobic)	Balakrishnan et al, 2004a	$\text{O}=\text{CH}-\text{CH}=\text{O}$
		<i>Clostridium sp. EDB2</i> , Isolated and Purified Enzyme	Bhushan et al., 2005	
		Nitroreductase from <i>Escherichia coli</i>	Bhushan et al., 2004a	
		<i>Phanerochaete chrysosporium</i>	Fournier et al., 2006	
		Photolysis	Hawari et al., 2004	
		Soil	Kuperman et al., 2006b	
7782-94-7	Nitramide (H <sub>2</sub> N <sub>2</sub> O <sub>2</sub> )	<i>Clostridium sp. EDB2</i> , Isolated and Purified Enzyme	Bhushan et al., 2005	$\begin{array}{c} \text{O} \\    \\ \text{O}=\text{N}-\text{NH}_2 \end{array}$
14797-55-8	Nitrate (NO <sub>3</sub> <sup>-</sup> )	Glass, Aqueous (Oxic)	Monteil-Rivera et al., 2004a	$\begin{array}{c} \text{O} \\    \\ \text{O}=\text{N}-\text{NH}_2 \end{array}$
		Hectorite	Szecsody et al., 2004	
		Photolysis	Hawari et al., 2004	
		Soil	Kuperman et al., 2006b	

**Table 4-2. Environmental Degradation Products of CL-20 (Continued)**

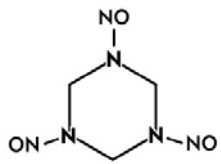
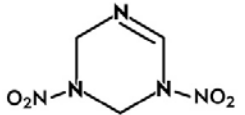
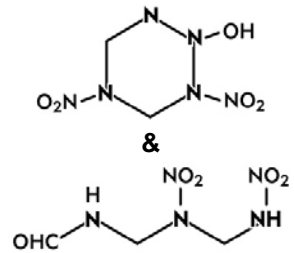
CASRN	Degradation Product (Chemical Formula)	Agent (Conditions)	Reference	Chemical Structure
14797-65-0	Nitrite (NO <sub>2</sub> <sup>-</sup> )	Alkaline Hydrolysis (pH 10)	Balakrishnan et al., 2003	$O=N-O^-$
		Alkaline Hydrolysis (pH 9.5)	Szecsody et al., 2004	
		<i>Clostridium sp. EDB2</i> , Isolated and Purified Enzyme	Bhushan et al., 2005	
		<i>Clostridium sp. EDB2</i> , Marine Isolate (Anaerobic)	Bhushan et al., 2004c	
		Glass, Aqueous (Oxic)	Monteil-Rivera et al., 2004a	
		Hectorite	Szecsody et al., 2004	
		Manganese Peroxidase (MnP)	Fournier et al., 2006	
		Nitroreductase from <i>Escherichia coli</i>	Bhushan et al., 2004a	
		Photolysis	Hawari et al., 2004	
		<i>Pseudomonas sp.</i> Strain FA1, Membrane-Enzyme Preparation	Bhushan et al., 2003a	
		Salicylate 1-Monooxygenase from <i>Pseudomonas sp.</i> Strain ATCC29352	Bhushan et al. 2004b	
		Soil	Kuperman et al., 2006b	
		Subsurface Sediment, Burbank (Oxic)	Szecsody et al., 2004	
		Subsurface Sediment, Norborne (Oxic)	Szecsody et al., 2004	
		Subsurface Sediment, Norborne (Reduced)	Szecsody et al., 2004	
		Subsurface Sediment, Ocala (Oxic)	Szecsody et al., 2004	
		Zero Valent Iron (Fe <sup>0</sup> ) (Anaerobic)	Balakrishnan et al, 2004a	
7727-37-9	Nitrogen (N <sub>2</sub> )	Photolysis	Hawari et al., 2004	$N \equiv N$
		Zero Valent Iron (Fe <sup>0</sup> ) (Anaerobic)	Balakrishnan et al., 2004a	
10024-97-2	Nitrous Oxide (N <sub>2</sub> O)	Alkaline Hydrolysis (pH 10)	Balakrishnan et al., 2003	$O=N \equiv N$
		<i>Clostridium sp. EDB2</i> , Isolated and Purified Enzyme	Bhushan et al., 2005	
		<i>Clostridium sp. EDB2</i> , Marine Isolate (Anaerobic)	Bhushan et al., 2004c	
		Glass, Aqueous (Oxic)	Monteil-Rivera et al., 2004a	
		<i>Irpex lacteus</i> (Aerobic)	Fournier et al., 2006	
		Nitroreductase from <i>Escherichia coli</i>	Bhushan et al., 2004a	
		<i>Phanerochaete chrysosporium</i> (Aerobic)	Fournier et al., 2006	
		Photolysis	Hawari et al., 2004	
		<i>Pseudomonas sp.</i> Strain FA1, Membrane-Enzyme Preparation	Bhushan et al., 2003a	
		Salicylate 1-Monooxygenase from <i>Pseudomonas sp.</i> Strain ATCC29352	Bhushan et al. 2004b	
		Soil	Kuperman et al., 2006b	
		Zero Valent Iron (Fe <sup>0</sup> ) (Anaerobic)	Balakrishnan et al, 2004a	

**Table 4-3. Environmental Degradation Products of Hexahydro-1,3,5-Triazine (RDX)**


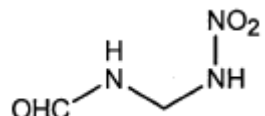
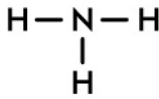



CASRN	Degradation Product (Chemical Formula)	Agent (Conditions)	Reference	Chemical Structure
5755-27-1	C <sub>3</sub> H <sub>6</sub> N <sub>6</sub> O <sub>5</sub> (Hexahydro-1-Nitroso-3,5-Dinitro-1,3,5-Triazine) (MNX)	Bacteria from Industrial Sludge, <i>HAW-1</i> (Anaerobic)	Zhao et al., 2003a	<p>The chemical structure of MNX is a six-membered ring with alternating carbon and nitrogen atoms. The top nitrogen atom is bonded to a nitroso group (NO), and the two bottom nitrogen atoms are each bonded to a nitro group (NO<sub>2</sub>).</p>
		Bacteria from Industrial Sludge, <i>HAW-1</i> , <i>HAW-HC1</i> , <i>HAW-E3</i> , <i>HAW-G4</i> , & <i>HAW-ES2</i> (Anaerobic)	Zhao et al., 2003b	
		<i>Klebsiella pneumoniae</i> strain <i>SCZ-1</i> (Anaerobic)	Zhao et al., 2002	
		Nitrate Reductase from <i>Aspergillus niger</i> , <i>Enerobacteriaceae</i> family (Anaerobic)	Bhushan et al., 2002	
		Non-Sterile Agricultural Topsoil (Anaerobic)	Sheremata et al., 2001	
		Psychrophilic Bacteria from Marine Sediment, <i>HAW-EB1</i> , <i>HAW-EB2</i> , <i>HAW-EB3</i> , <i>HAW-EB4</i> & <i>HAW-EB5</i> (Aerobic)	Zhao et al., 2004	
		Psychrophilic Bacteria from Marine Sediment, <i>HAW-EB17</i> , <i>HAW-EB18</i> & <i>HAW-EB21</i> (Anaerobic)	Zhao et al., 2004	
		Sludge (Anaerobic)	Halasz et al., 2002b	
		Tropical Marine Sediment Bacteria, <i>HAW-OC2</i> , <i>HAW-OC4</i> , & <i>HAW-OC6</i> (Anaerobic)	Bhatt et al., 2005	
80251-29-2	C <sub>3</sub> H <sub>6</sub> N <sub>6</sub> O <sub>4</sub> (Hexahydro-1,3-Dinitroso-5-Nitro-1,3,5-Triazine) (DNX)	Bacteria from Industrial Sludge, <i>HAW-1</i> (Anaerobic)	Zhao et al., 2003a	<p>The chemical structure of DNX is a six-membered ring with alternating carbon and nitrogen atoms. The top and bottom nitrogen atoms are each bonded to a nitroso group (NO), and the middle nitrogen atom is bonded to a nitro group (NO<sub>2</sub>).</p>
		Bacteria from Industrial Sludge, <i>HAW-1</i> , <i>HAW-HC1</i> , <i>HAW-E3</i> , <i>HAW-G4</i> , & <i>HAW-ES2</i> (Anaerobic)	Zhao et al., 2003b	
		Non-Sterile Agricultural Topsoil (Anaerobic)	Sheremata et al., 2001	

**Table 4-3. Environmental Degradation Products of RDX (Continued)**

CASRN	Degradation Product (Chemical Formula)	Agent (Conditions)	Reference	Chemical Structure
13980-04-6	$C_3H_6N_6O_3$ (Hexahydro-1,3,5-Trinitroso-1,3,5-Triazine) (TNX)	Psychrophilic Bacteria from Marine Sediment, <i>HAW-EB1</i> , <i>HAW-EB2</i> , <i>HAW-EB3</i> , <i>HAW-EB4</i> & <i>HAW-EB5</i> (Aerobic)	Zhao et al., 2004	
		Psychrophilic Bacteria from Marine Sediment, <i>HAW-EB17</i> , <i>HAW-EB18</i> & <i>HAW-EB21</i> (Anaerobic)	Zhao et al., 2004	
		Tropical Marine Sediment Bacteria, <i>HAW-OC2</i> , <i>HAW-OC4</i> , & <i>HAW-OC6</i> (Anaerobic)	Bhatt et al., 2005	
		Bacteria from Industrial Sludge, <i>HAW-1</i> (Anaerobic)	Zhao et al., 2003a	
		Bacteria from Industrial Sludge, <i>HAW-1</i> , <i>HAW-HC1</i> , <i>HAW-E3</i> , <i>HAW-G4</i> , & <i>HAW-ES2</i> (Anaerobic)	Zhao et al., 2003b	
178064-26-1	$C_3H_5N_5O_4$ pentahydro-3,5-1,3,5-triazacyclohex-1-ene	Non-Sterile Agricultural Topsoil (Anaerobic)	Sheremata et al., 2001	
		Psychrophilic Bacteria from Marine Sediment, <i>HAW-EB1</i> , <i>HAW-EB2</i> , <i>HAW-EB3</i> , <i>HAW-EB4</i> & <i>HAW-EB5</i> (Aerobic)	Zhao et al., 2004	
		Psychrophilic Bacteria from Marine Sediment, <i>HAW-EB17</i> , <i>HAW-EB18</i> & <i>HAW-EB21</i> (Anaerobic)	Zhao et al., 2004	
479422-93-0 & None	$C_3H_7N_5O_5$ (Carbinol of the Enamine & Ring Cleavage Product)	Alkaline Hydrolysis (pH 10)	Balakrishnan et al. 2003	
		Photolysis	Hawari et al., 2002	

**Table 4-3. Environmental Degradation Products of RDX (Continued)**

CASRN	Degradation Product (Chemical Formula)	Agent (Conditions)	Reference	Chemical Structure
10466-81-6	CH <sub>4</sub> N <sub>4</sub> O <sub>4</sub> (Methylenedinitramine) (MEDINA)	<i>Klebsiella pneumoniae</i> Strain SCZ-1 (Anaerobic)	Zhao et al., 2002	
		Nitrate Reductase from <i>Aspergillus niger</i> , <i>Enerobacteriaceae</i> family (Anaerobic)	Bhushan et al., 2002	
		Photolysis	Hawari et al., 2002	
		Psychrophilic Bacteria from Marine Sediment, <i>HAW-EB1</i> , <i>HAW-EB2</i> , <i>HAW-EB3</i> , <i>HAW-EB4</i> & <i>HAW-EB5</i> (Aerobic)	Zhao et al., 2004	
		Sludge (Anaerobic)	Halasz et al., 2002b	
		Tropical Marine Sediment Bacteria, <i>HAW-OC2</i> , <i>HAW-OC4</i> , & <i>HAW-OC6</i> (Anaerobic)	Bhatt et al., 2005	
None	C <sub>2</sub> H <sub>5</sub> N <sub>3</sub> O <sub>3</sub> (4-Nitro-2,4-Diazabutanal) (4-NDAB)	Alkaline Hydrolysis (pH 10)	Balakrishnan et al. 2003	
		Photolysis	Hawari et al., 2002	
		Psychrophilic Bacteria from Marine Sediment, <i>HAW-EB1</i> , <i>HAW-EB2</i> , <i>HAW-EB3</i> , <i>HAW-EB4</i> & <i>HAW-EB5</i> (Aerobic)	Zhao et al., 2004	
		<i>Rhodococcus sp.</i> Strain DN22 (Aerobic)	Bhushan et al. 2003b	
		<i>Rhodococcus sp.</i> Strain DN22 (Aerobic)	Fournier et al., 2002	
		<i>Rhodococcus sp.</i> Strain DN22 (Aerobic)	Fournier et al., 2004	
7664-41-7	Ammonia (NH <sub>3</sub> )	Alkaline Hydrolysis (pH 10)	Balakrishnan et al. 2003	
		Nitrate Reductase from <i>Aspergillus niger</i> , <i>Enerobacteriaceae</i> family (Anaerobic)	Bhushan et al., 2002	
		Photolysis	Hawari et al., 2002	
		<i>Rhodococcus sp.</i> Strain DN22 (Aerobic)	Fournier et al., 2002	
124-38-9	Carbon Dioxide (CO <sub>2</sub> )	Bacteria from Industrial Sludge, <i>HAW-1</i> (Anaerobic)	Zhao et al., 2003a	
		<i>Klebsiella pneumoniae</i> Strain SCZ-1 (Anaerobic)	Zhao et al., 2002	
		Non-Sterile Agricultural Topsoil (Anaerobic)	Sheremata et al., 2001	
		<i>Phanerochaete chrysosporium</i> (Liquid Culture)	Fournier et al., 2004	


**Table 4-3. Environmental Degradation Products of RDX (Continued)**

CASRN	Degradation Product (Chemical Formula)	Agent (Conditions)	Reference	Chemical Structure
		Psychrophilic Bacteria from Marine Sediment, <i>HAW-EB1</i> , <i>HAW-EB2</i> , <i>HAW-EB3</i> , <i>HAW-EB4</i> & <i>HAW-EB5</i> (Aerobic)	Zhao et al., 2004	
		Psychrophilic Bacteria from Marine Sediment, <i>HAW-EB17</i> , <i>HAW-EB18</i> & <i>HAW-EB21</i> (Anaerobic)	Zhao et al., 2004	
		<i>Rhodococcus sp.</i> Strain <i>DN22</i> (Aerobic)	Fournier et al., 2002	
		<i>Rhodococcus sp.</i> Strain <i>DN22</i> (Aerobic)	Fournier et al., 2004	
		Sludge (Anaerobic)	Halasz et al., 2002b	
		Tropical Marine Sediment Bacteria, <i>HAW-OC2</i> , <i>HAW-OC4</i> , & <i>HAW-OC6</i> (Anaerobic)	Bhatt et al., 2005	
50-00-0	Formaldehyde (CH <sub>2</sub> O)	Alkaline Hydrolysis (pH 10)	Balakrishnan et al. 2003	H <sub>2</sub> C=O
		Bacteria from Industrial Sludge, <i>HAW-1</i> (Anaerobic)	Zhao et al., 2003a	
		Bacteria from Industrial Sludge, <i>HAW-1</i> , <i>HAW-HC1</i> , <i>HAW-E3</i> , <i>HAW-G4</i> , & <i>HAW-ES2</i> (Anaerobic)	Zhao et al., 2003b	
		<i>Klebsiella pneumoniae</i> Strain <i>SCZ-1</i> (Anaerobic)	Zhao et al., 2002	
		<i>Nitrate Reductase</i> from <i>Aspergillus niger</i> , <i>Enerobacteriaceae</i> family (Anaerobic)	Bhushan et al., 2002	
		<i>Photolysis</i>	Hawari et al., 2002	
		<i>Rhodococcus sp.</i> Strain <i>DN22</i> (Aerobic)	Fournier et al., 2002	
		Sludge (Anaerobic)	Halasz et al., 2002b	
		Tropical Marine Sediment Bacteria, <i>HAW-OC2</i> , <i>HAW-OC4</i> , & <i>HAW-OC6</i> (Anaerobic)	Bhatt et al., 2005	
75-12-7	Formamide (CH <sub>3</sub> NO)	Photolysis	Hawari et al., 2002	H <sub>2</sub> N—CH=O
64-18-6	Formic acid (CH <sub>2</sub> O <sub>2</sub> )	Alkaline Hydrolysis (pH 10)	Balakrishnan et al. 2003	O=CH—OH
		Photolysis	Hawari et al., 2002	
67-56-1	Methanol (CH <sub>4</sub> O)	Bacteria from Industrial Sludge, <i>HAW-1</i> (Anaerobic)	Zhao et al., 2003a	H <sub>3</sub> C—OH

**Table 4-3. Environmental Degradation Products of RDX (Continued)**

CASRN	Degradation Product (Chemical Formula)	Agent (Conditions)	Reference	Chemical Structure
7782-94-7	Nitramide ( $\text{H}_2\text{N}_2\text{O}_2$ )	Bacteria from Industrial Sludge, <i>HAW-1</i> , <i>HAW-HC1</i> , <i>HAW-E3</i> , <i>HAW-G4</i> , & <i>HAW-ES2</i> (Anaerobic)	Zhao et al., 2003b	$\begin{array}{c} \text{O} \\    \\ \text{O}=\text{N}-\text{NH}_2 \end{array}$
		<i>Klebsiella pneumoniae</i> Strain <i>SCZ-1</i> (Anaerobic)	Zhao et al., 2002	
		<i>Klebsiella pneumoniae</i> Strain <i>SCZ-1</i> (Anaerobic)	Zhao et al., 2002	
		<i>Rhodococcus sp.</i> Strain <i>DN22</i> (Aerobic)	Fournier et al., 2004	
		Sludge (Anaerobic)	Halasz et al., 2002b	
14797-55-8	Nitrate ( $\text{NO}_3^-$ )	Photolysis	Hawari et al., 2002	$\begin{array}{c} \text{O} \\    \\ \text{O}=\text{N}-\text{O}^- \end{array}$
14797-65-0	Nitrite ( $\text{NO}_2^-$ )	Alkaline Hydrolysis (pH 10)	Balakrishnan et al. 2003	$\text{O}=\text{N}-\text{O}^-$
		Bacteria from Industrial Sludge, <i>HAW-1</i> (Anaerobic)	Zhao et al., 2003a	
		Photolysis	Hawari et al., 2002	
		Psychrophilic Bacteria from Marine Sediment, <i>HAW-EB1</i> , <i>HAW-EB2</i> , <i>HAW-EB3</i> , <i>HAW-EB4</i> & <i>HAW-EB5</i> (Aerobic)	Zhao et al., 2004	
		<i>Rhodococcus sp.</i> Strain <i>DN22</i> (Aerobic)	Fournier et al., 2002	

**Table 4-3. Environmental Degradation Products of RDX (Continued)**

CASRN	Degradation Product (Chemical Formula)	Agent (Conditions)	Reference	Chemical Structure
10024-97-2	Nitrous Oxide (N <sub>2</sub> O)	Alkaline Hydrolysis (pH 10)	Balakrishnan et al. 2003	
		Bacteria from Industrial Sludge, <i>HAW-1</i> (Anaerobic)	Zhao et al., 2003a	
		Bacteria from Industrial Sludge, <i>HAW-1</i> , <i>HAW-HC1</i> , <i>HAW-E3</i> , <i>HAW-G4</i> , & <i>HAW-ES2</i> (Anaerobic)	Zhao et al., 2003b	
		<i>Klebsiella pneumoniae</i> Strain <i>SCZ-1</i> (Anaerobic)	Zhao et al., 2002	
		Nitrate Reductase from <i>Aspergillus niger</i> , <i>Enerobacteriaceae</i> family (Anaerobic)	Bhushan et al., 2002	
		Non-Sterile Agricultural Topsoil (Anaerobic)	Sheremata et al., 2001	
		Phanerochaete chrysosporium ( Liquid Culture)	Fournier et al., 2004	
		Photolysis	Hawari et al., 2002	
		Psychrophilic Bacteria from Marine Sediment, <i>HAW-EB1</i> , <i>HAW-EB2</i> , <i>HAW-EB3</i> , <i>HAW-EB4</i> & <i>HAW-EB5</i> (Aerobic)	Zhao et al., 2004	
		<i>Rhodococcus sp.</i> Strain <i>DN22</i> (Aerobic)	Fournier et al., 2002	
		Sludge (Anaerobic)	Halasz et al., 2002b	
		Tropical Marine Sediment Bacteria, <i>HAW-OC2</i> , <i>HAW-OC4</i> , & <i>HAW-OC6</i> (Anaerobic)	Bhatt et al., 2005	



Both formaldehyde (Thompson et al., 2005) and glyoxal (Crocker et al., 2005) will mineralize to form CO<sub>2</sub>, and mineralization will be rapid in moist soil and aqueous environments (IPCS 2004, ATSDR, 1999).

Table 4-4 lists the environmental breakdown of products of TNT. Many of them are toluene derivatives, unlike the degradation products of CL-20 and RDX. Aside from nitrate, TNT does not appear to have any degradation products in common with CL-20 or RDX. In addition, TNT differs from both CL-20 and RDX because:

- Complete mineralization of TNT is not likely in the environment
- Many of the breakdown products of TNT are relatively toxic and will persist for substantial periods in environmental media
- Degradation of TNT may produce a polymer that has yet to be fully characterized (Hawari et al., 1998).

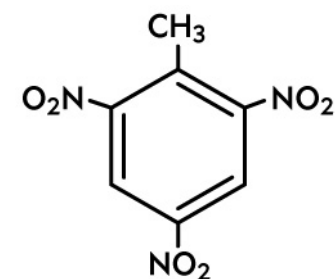
Comparing Tables 4-2, 4-3 and 4-4 clearly indicates that CL-20 and RDX are much more similar to each other than they are to TNT in terms of the persistence and toxicities of their likely degradation products.

The results summarized in Tables 4-2 and 4-3 indicate that CL-20 and RDX may differ in their environmental degradation end products by the potential formation of glyoxal from CL-20 compared to the formation of formaldehyde from RDX. The toxicities of glyoxal and formaldehyde have been studied extensively. For example, see reviews by Shangari et al. (2003) and IPCS (2004) on glyoxal and ATSDR (1999) on formaldehyde.

Glyoxal is produced endogenously from sugars in the body and is normally effectively detoxified to form glycolate (Shangari et al., 2003; ICPS, 2004). It is also often detected in fermented foods and beverages—including beer, wine, yogurt, and bread—and is released to the air by residential wood combustion (ICPS, 2004). The main sources of glyoxal exposure for the general population are most likely food and drinking water.

In the environment, glyoxal is usually found in the hydrosphere and in soil, and to a lesser extent in air (IPCS, 2004). Glyoxal in soil may leach to groundwater ( $\log K_{oc} < 1$ ), but would be expected to readily biodegrade. It appears to be a tumor promoter and has been shown to be mutagenic in cell culture test systems, although the latter effect was reduced by adding metabolic enzymes (S9) to the systems (Shangari et al., 2003).

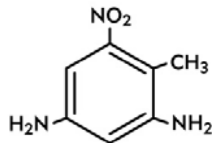
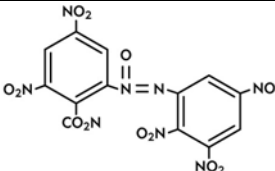
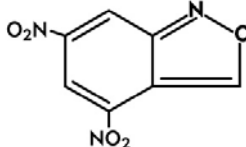
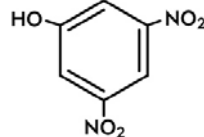
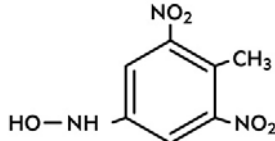
Shangari et al. (2003) suggested that diets poor in thiamine and high in sugars could result in increased levels of endogenous glyoxals (glyoxal and methylglyoxal). Further, based on the results of a study on rats fed a sucrose-based, thiamine-deficient diet, they suggested that elevated endogenous glyoxal or exposures to glyoxal from exogenous sources could lead to increased risk of colon cancer. However, this hypothesis remains speculative and would require substantial additional testing to determine whether human health might be adversely affected by long-term, low-level exposures to glyoxal in soil and water and, if so, at what concentrations or doses.



**Table 4-4. Environmental Degradation Products of 2,4,6-Trinitrotoluene (TNT)**

CASRN	Degradation Product (Chemical Formula)	Agent (Conditions)	Reference	Chemical Structure
19406-51-0	Amino-2,6-Dinitrotoluene, 4- (C <sub>7</sub> H <sub>7</sub> N <sub>3</sub> O <sub>4</sub> ) (4-ADNT)	Microbial Decomposition	Becker, 1995	<p>Chemical structure of Amino-2,6-Dinitrotoluene, 4- (4-ADNT): A benzene ring with a methyl group (CH<sub>3</sub>) at position 1, an amino group (H<sub>2</sub>N) at position 4, and nitro groups (NO<sub>2</sub>) at positions 2 and 6.</p>
		Photolysis	Becker, 1995	
		Sludge & Molasses (Anaerobic)	Hawari et al., 1998	
		Surface and Subsurface Soil from TNT Manufacturing Plant	Halasz et al., 2002a	
		Water in Ditch from TNT Manufacturing Plant	Halasz et al., 2002a	
140380-55-8	Amino-4,6-Dinitrobenzoic Acid, 2- (C <sub>7</sub> H <sub>5</sub> N <sub>3</sub> O <sub>6</sub> )	Photolysis	Becker, 1995; Brannon & Pennington, 2002	<p>Chemical structure of Amino-4,6-Dinitrobenzoic Acid, 2-: A benzene ring with a carboxylic acid group (CO<sub>2</sub>H) at position 1, an amino group (NH<sub>2</sub>) at position 2, and nitro groups (NO<sub>2</sub>) at positions 4 and 6.</p>
35572-78-2	Amino-4,6-Dinitrotoluene, 2- (C <sub>7</sub> H <sub>7</sub> N <sub>3</sub> O <sub>4</sub> ) (2-ADNT)	Microbial Decomposition	Becker, 1995	<p>Chemical structure of Amino-4,6-Dinitrotoluene, 2- (2-ADNT): A benzene ring with a methyl group (CH<sub>3</sub>) at position 1, an amino group (NH<sub>2</sub>) at position 2, and nitro groups (NO<sub>2</sub>) at positions 4 and 6.</p>
		Sludge & Molasses (Anaerobic)	Hawari et al., 1998	
		Surface and Subsurface Soil from TNT Manufacturing Plant	Halasz et al., 2002a	
		Water in Ditch from TNT Manufacturing Plant	Halasz et al., 2002a	
None	Carboxy-3,3',5,5'-Tetranitroazoxybenzene, 2-	Photolysis	Becker, 1995	
None	Carboxy-3,3',5,5'-Tetranitro-NNO-Azoxybenzene, 2-	Photolysis	Brannon & Pennington, 2002	
59229-75-3	Diamino-4-Nitrotoluene, 2,6- (C <sub>7</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub> ) (2,6-DANT)	Microbial Decomposition	Becker, 1995	<p>Chemical structure of Diamino-4-Nitrotoluene, 2,6- (2,6-DANT): A benzene ring with a methyl group (CH<sub>3</sub>) at position 1, nitro groups (NO<sub>2</sub>) at positions 2 and 6, and amino groups (NH<sub>2</sub>) at positions 3 and 5.</p>
		Sludge & Molasses (Anaerobic)	Hawari et al., 1998	

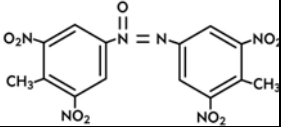
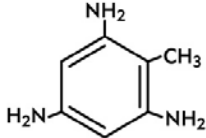
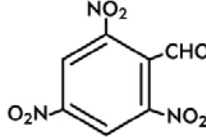
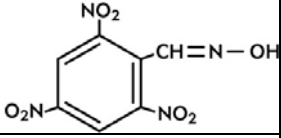
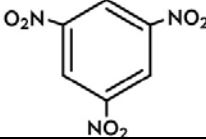
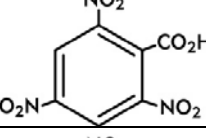
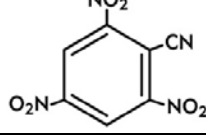
**Table 4-4. Environmental Degradation Products of TNT (Continued)**

CASRN	Degradation Product (Chemical Formula)	Agent (Conditions)	Reference	Chemical Structure
6629-29-4	Diamino-6-Nitrotoluene, 2,4'- (C <sub>7</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub> ) (2,4-DANT)	Microbial Decomposition	Becker, 1995	
		Sludge & Molasses (Anaerobic)	Hawari et al., 1998	
None	Diaminonitrotoluene (C <sub>7</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub> )	Microbial Decomposition	Becker, 1995	
None	Dicarboxy-3,3',5,5'- Tetranitroazobenzene, 2,2'-	Photolysis	Becker, 1995; Brannon & Pennington, 2002	
4276-95-3	Dicarboxy-3,3',5,5'- Tetranitroazoxybenzene, 2,2'- (C <sub>14</sub> H <sub>6</sub> N <sub>6</sub> O <sub>13</sub> )	Photolysis	Becker, 1995; Brannon & Pennington, 2002	
None	Dimethyl-3,3',5,5'-Tetranitro- ONN-Azoxybenzene, 2,4'-	Photolysis	Becker, 1995; Brannon & Pennington, 2002	
None	Dimethyl-3,3',5,5'-Tetranitro- ONN-Azoxybenzene, 2',4-	Photolysis	Becker, 1995; Brannon & Pennington, 2002	
29245-51-0	Dinitroanthranil, 4,6- (C <sub>7</sub> H <sub>3</sub> N <sub>3</sub> O <sub>5</sub> )	Photolysis	Becker, 1995; Brannon & Pennington, 2002	
None	Dinitroisoanthranil, 4,6-	Photolysis	Becker, 1995; Brannon & Pennington, 2002	
586-11-8	Dinitrophenol, 3,5- (C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> O <sub>5</sub> ) (3,5-DNP)	Photolysis	Becker, 1995; Brannon & Pennington, 2002	
None	Dinitrosoanthranil, 2,4'-	Photolysis	Brannon & Pennington, 2002	
59283-75-9	Hydroxylamino-2,6- Dinitrotoluene, 4- (C <sub>7</sub> H <sub>7</sub> N <sub>3</sub> O <sub>5</sub> ) (4- HADNT)	Microbial Decomposition	Becker, 1995	
		Sludge & Molasses (Anaerobic)	Hawari et al., 1998	

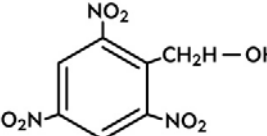
**Table 4-4. Environmental Degradation Products of TNT (Continued)**

CASRN	Degradation Product (Chemical Formula)	Agent (Conditions)	Reference	Chemical Structure
59283-76-0	Hydroxylamino-4,6-Dinitrotoluene, 2- ( $C_7H_7N_3O_5$ ) (2-HADNT)	Sludge & Molasses (Anaerobic)	Hawari et al., 1998	
None	Monoaminodinitrotoluene	Microbial Decomposition	Becker, 1995	
None	N-(2-Carboxy-3,5-Dinitrophenyl)-2,4,6-Trinitrobenzamide	Photolysis	Becker, 1995; Brannon & Pennington, 2002	
14797-55-8	Nitrate ( $NO_3^-$ )	Microbial Decomposition	Becker, 1995	
None	Polymers	Sludge & Molasses (Anaerobic; pH 7.2)	Hawari et al., 1998	
None	Tetraamino-4,4'-Azotoluene, 2,2',6,6' - (2,2',6,6'-TA-4,4'-azoT),	Sludge & Molasses (Anaerobic; pH 7.2)	Hawari et al., 1998	
None	Tetraamino-6,6'-Azotoluene, 2,2',4,4' - (2,2',4,4'-TA-6,6'-azoT)	Sludge & Molasses (Anaerobic; pH 7.2)	Hawari et al., 1998	
35212-01-2	Tetranitro-2,2'-Azoxytoluene, 4,4',6,6' - ( $C_{14}H_{10}N_6O_9$ ) (2,2'-Az)	Microbial Decomposition	Becker, 1995	
		Photolysis	Becker, 1995; Brannon & Pennington, 2002	

**Table 4-4. Environmental Degradation Products of TNT (Continued)**

CASRN	Degradation Product (Chemical Formula)	Agent (Conditions)	Reference	Chemical Structure
51857-25-1	Tetranitro-4,4'-Azoxytoluene, 2,2',6,6'- (C <sub>14</sub> H <sub>10</sub> N <sub>6</sub> O <sub>9</sub> ) (4,4'-Az)	Microbial Decomposition	Becker, 1995	
		Photolysis	Becker, 1995; Brannon & Pennington, 2002	
None	Tetranitro-4-Azoxytoluene, 2,2',6,6'- (4-Az)	Microbial Decomposition	Becker, 1995	
		Microbial Decomposition	Becker, 1995	
88-02-8	Triaminotoluene, 2,4,6- (C <sub>7</sub> H <sub>11</sub> N <sub>3</sub> ) (2,4,6-TAT)	Microbial Decomposition	Becker, 1995	
		Sludge & Molasses (Anaerobic)	Hawari et al., 1998	
606-34-8	Trinitrobenzaldehyde, 2,4,6- (C <sub>7</sub> H <sub>3</sub> N <sub>3</sub> O <sub>7</sub> ) (TNBAL)	Photolysis	Becker, 1995; Brannon & Pennington, 2002	
42449-44-5	Trinitrobenzaldoxime, 2,4,6- (C <sub>7</sub> H <sub>4</sub> N <sub>4</sub> O <sub>7</sub> )	Photolysis	Becker, 1995; Brannon & Pennington, 2002	
99-35-4	Trinitrobenzene, 1,3,5- (C <sub>6</sub> H <sub>3</sub> N <sub>3</sub> O <sub>6</sub> ) (1,3,5-TNB)	Photolysis	Becker, 1995; Brannon & Pennington, 2002	
129-66-8	Trinitrobenzoic Acid, 2,4,6- (C <sub>7</sub> H <sub>3</sub> N <sub>3</sub> O <sub>8</sub> ) (TNBA)	Photolysis	Becker, 1995; Brannon & Pennington, 2002	
37841-25-1	Trinitrobenzonitrile, 2,4,6- (C <sub>7</sub> H <sub>2</sub> N <sub>4</sub> O <sub>6</sub> )	Photolysis	Becker, 1995; Brannon & Pennington, 2002	

**Table 4-4. Environmental Degradation Products of TNT (Continued)**

CASRN	Degradation Product (Chemical Formula)	Agent (Conditions)	Reference	Chemical Structure
24577-68-2	Trinitrobenzyl Alcohol, 2,4,6- (C <sub>7</sub> H <sub>5</sub> N <sub>3</sub> O <sub>7</sub> ) (TNBOH)	Photolysis	Becker, 1995; Brannon & Pennington, 2002	

Formaldehyde, too, is produced endogenously in the body and is normally rapidly detoxified by most—if not all—cells, tissues, and organs (ATSDR, 1999). Combustion sources, including power plants, incinerators, refineries, cigarettes, and forest fires account for most of the formaldehyde entering the environment, and most exposures are via inhalation because formaldehyde typically dissolves and degrades rapidly in aqueous media. However, the fate of formaldehyde in soil has not yet been adequately determined (ATSDR, 1999).

Thus, the available information is not adequate to determine whether glyoxal from CL-20 would pose a greater threat (if any) to human health or the environment than formaldehyde from RDX.

Table 4-5 lists thermal degradation products that have been associated with the combustion or explosion of CL-20, RDX, and TNT in the available literature. Unlike RDX and TNT, polycyclic aromatic hydrocarbons (PAHs) have not been reported as thermal degradation products of CL-20 in the available literature. However, it is reasonable to assume that the thermal degradation of CL-20 yields the same or similar PAHs.

Unlike RDX and TNT, the thermal breakdown of CL-20 yields isocyanic acid (Table 4-5). Like hydrogen cyanide, which is produced by both CL-20 and RDX, isocyanic acid is a highly toxic gas. However, both isocyanic acid and hydrogen cyanide would be expected to rapidly dissipate in air after an explosion and would be expected to represent no acute threat to human health or the environment outside the boundaries of the physical damage caused by the explosion, as well as no significant inhalation exposures inside these boundaries after the blast.

On the other hand, the thermal breakdown of CL-20 results in an amorphous solid residue not reported after the breakdown of either RDX or TNT. The residue contains a compound that appears to have the chemical formula  $C_3H_3N_2O_2$ . However, neither the chemical structure of this compound nor the other constituents of the residue have yet been determined. Thus, the information is inadequate to determine whether the residue or its constituents may pose a threat to human health or the environment.

### **4.3 Environmental Transport of CL-20, RDX and TNT**

The mobility of an energetic chemical depends substantially on environmental conditions, the physicochemical properties of the chemical under those conditions, and the form and nature of the released material containing the chemical.

Because mobility is influenced by a wide range of factors, there are a large number of possible environmental scenarios. Attempting to quantify the amount and rate of transport of these energetic chemicals is neither possible nor meaningful for this report. Rather, the mobility of CL-20 and other energetic chemicals is qualitatively described.

#### **4.3.1 Mobility in Air**

As discussed in Section 4.1, CL-20 and the other common energetic chemicals have characteristically very low vapor pressures and are unlikely to be found as vapors in the environment. Thus, energetic chemicals in air will typically be found primarily in the form of particulate matter.

The most likely mechanism for release and transport of airborne CL-20 is detonation—especially low-order detonation—when small particles containing CL-20 from incomplete combustion may be released together with the thermal degradation products of CL-20 (Table 4-5).

**Table 4-5. Thermal Degradation Products of CL-20, RDX, and TNT**

CASRN	Degradation Product (Chemical Formula)	CL-20	RDX	TNT
7664-41-7	Ammonia (NH <sub>3</sub> )		Groom et al., 2003	
56-55-3	Benz(α)Anthracene (C <sub>18</sub> H <sub>12</sub> )		Becker, 1995	Becker, 1995
71-43-2	Benzene (C <sub>6</sub> H <sub>6</sub> )		Becker, 1995	Becker, 1995
50-32-8	Benzo(α)Pyrene (C <sub>20</sub> H <sub>12</sub> )		Becker, 1995	Becker, 1995
	C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> O <sub>2</sub> in an Amorphous Solid Residue*	Korsounskii et al., 2000		
		Korsounskii et al., 2000; Patil & Brill, 1993		
124-38-9	Carbon Dioxide (CO <sub>2</sub> )	Korsounskii et al., 2000; Patil & Brill, 1991, 1993; Loebbecke et al., 1998	Becker, 1995; Zhao et al., 1988	Becker, 1995
630-08-0	Carbon Monoxide (CO)	Patil & Brill, 1991, 1993	Becker, 1995; Zhao et al., 1988	Becker, 1995
132-64-9	Dibenzofuran (C <sub>12</sub> H <sub>8</sub> O)		Becker, 1995	Becker, 1995
121-14-2	Dinitrotoluene, 2,4- (C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>4</sub> ) (2,4-DNT)		Becker, 1995	Becker, 1995
606-20-2	Dinitrotoluene, 2,6- (C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>4</sub> ) (2,6-DNT)		Becker, 1995	Becker, 1995
122-39-4	Diphenylamine (C <sub>12</sub> H <sub>11</sub> N)		Becker, 1995	Becker, 1995
50-00-0	Formaldehyde (CH <sub>2</sub> O)		Halasz et al., 2002b; Groom et al., 2003; Zhao et al., 1988	
74-90-8	Hydrogen Cyanide (HCN)	Korsounskii et al., 2000; Patil & Brill, 1991, 1993; Loebbecke et al., 1998	Zhao et al., 1988	
75-13-8	Isocyanic Acid (HNCO)	Patil & Brill, 1991, 1993		
74-82-8	Methane (CH <sub>4</sub> )		Becker, 1995	Becker, 1995
91-20-3	Naphthalene (C <sub>10</sub> H <sub>8</sub> )		Becker, 1995	Becker, 1995
119-75-5	Nitrodiphenylamine, 2- (C <sub>12</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub> )		Becker, 1995	
7727-37-9	Nitrogen (N <sub>2</sub> )	Korsounskii et al., 2000	Halasz et al., 2002b	



**Table 4-5. Thermal Degradation Products of CL-20, RDX, and TNT (Continued)**

CASRN	Degradation Product (Chemical Formula)	CL-20	RDX	TNT
10102-44-0	Nitrogen Dioxide (NO <sub>2</sub> )	Korsounskii et al., 2000; Patil & Brill, 1991, 1993; Loebbecke et al., 1998	Becker, 1995; Zhao et al., 1988	Becker, 1995
10102-43-9	Nitrogen Oxide (NO)	Korsounskii et al., 2000; Patil & Brill, 1991, 1993	Becker, 1995; Zhao et al., 1988	Becker, 1995
581-89-5	Nitronaphthalene, 2- (C <sub>10</sub> H <sub>7</sub> NO <sub>2</sub> )		Becker, 1995	Becker, 1995
5522-43-0	Nitropyrene, 1- (C <sub>16</sub> H <sub>9</sub> NO <sub>2</sub> )		Becker, 1995	Becker, 1995
7782-77-6	Nitrous Acid (HNO <sub>2</sub> )	Patil & Brill, 1991	Zhao et al., 1988	
10024-97-2	Nitrous Oxide (N <sub>2</sub> O)	Korsounskii et al., 2000; Patil & Brill, 1991, 1993; Loebbecke et al., 1998	Halasz et al., 2002b; Groom et al., 2003; Balakrishnan et al., 2003; Zhao et al., 1988	
86-30-6	N-Nitrosodiphenylamine (C <sub>12</sub> H <sub>10</sub> N <sub>2</sub> O)		Becker, 1995	Becker, 1995
None	Non-Methane Hydrocarbons		Becker, 1995	Becker, 1995
108-95-2	Phenol (C <sub>6</sub> H <sub>6</sub> O)			Becker, 1995
129-00-0	Pyrene (C <sub>16</sub> H <sub>10</sub> )		Becker, 1995	Becker, 1995
99-35-4	Trinitrobenzene, 1,3,5- (C <sub>6</sub> H <sub>3</sub> N <sub>3</sub> O <sub>6</sub> ) (1,3,5-TNB)		Becker, 1995	Becker, 1995

 = Not Reported as a Thermal Degradation Product in the Available Literature

\*Residue & Structure of the Reported Constituent has not been Defined.

Becker (1995) reported the results of studies in which air samples were collected by passing samplers through explosive clouds after detonating RDX or TNT. Surface soil samples were also collected in the detonation areas after these explosions. In addition to the thermal degradation products listed in Table 4-5, traces of the parent compounds (TNT, 360 ppb; RDX, 15 ppb) were the most common contaminants found in the soil samples collected in the detonation zone. Similar air-release and deposition patterns may be expected for CL-20.

#### **4.3.2 Mobility in Surface Water**

The release of CL-20 and the other energetic chemicals to surface water largely depends on their solubilities. At 20°C, TNT has the highest solubility and is expected to be present at higher concentrations, all other factors being equal, while CL-20 generally has the lowest solubility of the four energetic chemicals examined.

Once dissolved in surface water, the mobility of an energetic chemical will generally not be temperature-dependent as long as the water remains liquid, even though the solubility and other physicochemical properties of the energetic chemical will vary with changes in temperature. This observation would be expected to apply to CL-20, as well as to RDX and TNT in water.

The distance that detectable CL-20 may migrate in surface water from a point source will depend on factors such as the dilution and degradation of CL-20 in the water. Dilution may be an important factor, especially in turbulent streams and rivers, and would be an equally important factor for CL-20, RDX, HMX, and TNT. In addition, photolysis is a common degradation mechanism in surface waters. The photolysis of CL-20 was found to be much more rapid than for RDX (Hawari et al., 2004b). Thus, all other factors being equal, photolysis may result in detectable RDX concentrations in water extending farther from the point of release compared with CL-20.

On the other hand, the rate of photolysis can vary substantially depending on environmental conditions and the characteristics of the water body. For example, under natural sunlight, RDX dissolved in water has an experimental half-life of about 10 hours, but the half-life reported for RDX in a wastewater lagoon ranged from 456 days to about 2,000 days, depending on the time of year and depth of the lagoon (ATSDR, 1995a).

#### **4.3.3 Mobility in Soil**

The mobility of an energetic chemical in soil will depend on a number of factors. First, the chemical preparation must decompose or disintegrate into smaller fragments, especially if it is present in particulate matter in UXO or over the ground surface after a low-order detonation. Next, the energetic chemical must dissolve into the water associated with the soil. Generally, it will move through the soil with the water fraction. However, the movement of the chemical through the soil may be impeded by sorption to organic matter, clays, or other substances in the soil. Furthermore, the distance that detectable concentrations of the chemical migrate from the source of the contamination may be limited by both abiotic and biotic environmental degradation processes. All of these factors—including dissolution rate, solubility, sorption, and environmental degradation—will depend, in turn, on environmental conditions and the composition and characteristics of the soil (e.g., temperature, pH, clay and organic matter content, moisture, porosity, microflora, and microfauna).

As noted in Section 4.1, the four energetic chemicals considered in this evaluation can be ranked based on their solubilities as follows: CL-20 < HMX < RDX < TNT. The relatively low solubility is expected to reduce the mobility of CL-20 in soil compared with that of RDX, HMX, and TNT.

Pennington et al. (2001) found that CL-20 was less stable in water than RDX and HMX and speculated that the lower stability of CL-20 was related to its inherently less stable chemical structure. Thus, once CL-20 is dissolved in the water associated with a soil, it may tend to degrade faster—as a result of its more labile chemical structure—than RDX and HMX.

CL-20 has a higher affinity for soils relative to RDX, and its mobility is expected to be somewhat attenuated by soils, especially those soils rich in organic matter (Balakrishnan et al., 2004b). CL-20 is readily biodegraded in soil (Trott et al., 2003), which should limit its mobility. In near surface soils, CL-20 is degraded slightly faster in reducing conditions compared to oxidizing conditions, but the difference is <10X. Tropical wet soils with abundant organic carbon most favor the sorption and degradation of CL-20, especially where photolysis can occur. The type, as well as the amount, of organic matter is important (Hawari et al., 2003).

Under aerobic conditions without organic soil amendments and without exposure to light, CL-20 showed virtually no degradation (Strigul et al., 2006). These latter conditions are likely to be common in locations where CL-20 might be used.

Jenkins et al. (2003) estimated the half-lives of CL-20, RDX, and HMX in three military training ranges maintained under moist, unsaturated conditions in the dark. CL-20 and RDX were found to be very similar, with half-lives in the range of 69–267 days for CL-20 and 94–154 days for RDX, while the half-life of HMX ranged from 133–2,310 days, depending upon soil type. The authors concluded that all three energetic chemicals have similar stabilities in soil, and that dissolved CL-20 would have degradation characteristics similar to RDX and HMX.

Szecsody et al. (2005) measured the half-lives of CL-20 and RDX in soil under aerobic and anaerobic conditions. These researchers found that the half-life of CL-20 under aerobic conditions in China Lake soils was 17 days in surface soil and 32 days in subsurface soils. The half-lives of RDX under these conditions were 5 days in surface soil and 693 days in subsurface soils. The pH of the China Lake soils was somewhat high (approximately 8.5), which may have accelerated degradation. Under anaerobic conditions, the half-lives of CL-20 and RDX were 12 and 2.3 days, respectively, in surface soil and 17 and 2.7 days, respectively, in subsurface soil. These data suggest that CL-20 is more persistent than RDX, except in aerobic subsurface soil.

Other authors have determined half-lives for RDX, HMX, and TNT that are much different from those discussed above. One of the earliest studies on the environmental fate of energetic chemicals was performed by DuBois and Baytos beginning in 1972 at the Los Alamos National Laboratory in New Mexico (DuBois and Baytos, 1991). After 20 years, over 70 percent of the RDX and HMX and only about 10 percent of TNT remained in the undisturbed forested location where they were buried. The half-lives of RDX, HMX, and TNT were determined to be 36 years, 39 years, and 1 year, respectively. The RDX data are consistent with Tucker et al. (1985), who determined that RDX had a half-life of 36 years by placing RDX in soil pots outdoors. The reported half-life for TNT varies, but literature values are typically in the range of 1 to 10 years.

RDX and HMX have solubilities that are much lower than that of TNT, but they are more mobile in saturated soils because TNT mobility is typically attenuated through sorption, transformation,

and abiotic degradation. Although TNT is relatively soluble and mobile, it has not been found in groundwater beneath ranges because TNT quickly becomes transformed or degraded before it reaches groundwater. Conversely, RDX and HMX are not readily bound or attenuated by soils, except perhaps by clays, and once dissolved, they are expected to migrate readily in groundwater unless anaerobic conditions are encountered. CL-20 has little or no affinity for clays but does sorb to certain types of organic matter (Balakrishnan et al., 2004b), and sorption in the subsurface is correlated with the mass of iron oxides (Szecsody et al., 2005). Although the mobility of CL-20 may be reduced somewhat in some soils rich in certain types of organic matter or iron oxides, the mobility of CL-20 is only slightly retarded through sorption.

CL-20 is degradable under a wider range of surface soil conditions relative to RDX. For example, the rates of CL-20 degradation are similar under oxidizing and reducing conditions. On the other hand, the rate of RDX degradation is about 3 orders of magnitude lower under oxidizing conditions relative to reducing conditions. CL-20 may generally be less persistent in the soils than RDX because CL-20 can be readily degraded under a wider range of environmental conditions.

In semi-arid and arid environments, energetic chemicals can persist for decades, especially if buried. Where rainfall is greater, energetic chemicals are more likely to be mobilized and transported through the soil and into groundwater.

In studies conducted in soils under unsaturated conditions, Szecsody et al. (2005) found that the sorption trends for CL-20 and RDX were similar in the three soil types tested (MSC, Norborne, and Burbank). More important, however, was the finding that the transport of CL-20 and RDX under unsaturated conditions with very low water content (<30 percent moisture saturation) was likely to be accelerated relative to values derived from saturated soil experiments. Low water content conditions may decrease the access of CL-20 and RDX molecules to surfaces and sites for sorption.

Relative to RDX, CL-20 is generally regarded as less stable and can be degraded under a wider range of environmental conditions. Under certain conditions (e.g., tropical, moist, organic-rich soils) the stability of CL-20 could be significantly less than RDX, while under reducing conditions, CL-20 may be significantly more stable than RDX. Nevertheless, the literature, in general, suggests that the stability of CL-20 and RDX should be considered similar.

#### **4.3.4 Mobility in Groundwater**

Although there are small differences in the soil  $K_d$ s for RDX and CL-20, neither of these energetic chemicals sorb strongly to soils, sediments, or aquifer materials. RDX and CL-20 are both likely to migrate at about the same rate as groundwater. Although the concentrations in groundwater may be low because of solubility limits, a CL-20 plume could be sustained as CL-20 slowly dissolves and small portions of CL-20 that were previously dissolved and sorbed onto aquifer materials desorb into groundwater.

CL-20 and RDX can be expected to behave similarly under most groundwater conditions. Where groundwater pH is elevated (pH>7.5) and CL-20 undergoes abiotic degradation, its transport is likely to be less extensive relative to RDX. Conversely, under reducing groundwater conditions, CL-20 transport is likely to extend farther than RDX, all other factors being equal.

Because the overall sorption of CL-20 on aquifer materials is only about 10 percent greater than RDX, there will be little practical difference in their sorption and retardation in groundwater (Szecsody et al., 2005). CL-20 is, therefore, likely to mimic the contaminant patterns found for

RDX and migrate deep into the subsurface soil and move nearly unretarded in groundwater (Szecsody et al., 2005). Abiotic processes (from the presence of ferrous iron and other transition metals) will be primarily responsible for CL-20 degradation in the deep subsurface where biological activity may be limited by the availability of electron donors. Degradation rates will range from weeks (in iron reducing systems) to years.

#### **4.3.5 Aging**

Crockett et al. (1999) reported that energetic chemicals in weathered, contaminated soils exhibited slower degradation and desorption kinetics than energetic residues in spiked soil samples. Although this work did not include CL-20, the findings are consistent with the more recent work by Szecsody et al. (2005), in which CL-20 and RDX were both found to strongly but slowly sorb to different soil components. RDX desorption was somewhat slower than that of CL-20.

Aging studies have also shown that CL-20, like many other substances, desorbs much more slowly with greater aging. This suggests that CL-20 is relatively immobile when sorbed and that sorbed CL-20 will undergo degradation at a slower rate and be more persistent in soils and in groundwater. Both CL-20 and RDX are likely to present similar groundwater concerns and have similar transport rates and mobility despite differences in aging and sorption characteristics.

### **4.4 Uptake and Bioaccumulation of CL-20, RDX, TNT, and Associated Substances in Biota**

The characteristics of CL-20, RDX, and TNT that are relevant to their uptake by plants and soil invertebrates and their availability for absorption in wildlife and humans are important for evaluating their relative risks. These MCs have similar, relatively low-to-moderate bioconcentration and bioaccumulation potential in various biota. The log  $k_{ow}$ s for CL-20, RDX, and TNT are 1.92, 0.87–0.90, and 1.6, respectively (Monteil-Rivera et al., 2004a; HSBD, [Cyclonite Full Record](#) and [2,4,6-Trinitrotoluene Full Record](#)), indicating low lipid solubility and, therefore, low likelihood of bioconcentration and bioaccumulation. However, low log  $k_{ow}$ s alone are insufficient to support a definitive statement that a substance is not likely to bioaccumulate. Thus, studies in plants, soil/sediment invertebrates, terrestrial wildlife, and aquatic/benthic organisms were consulted to find experimentally determined or estimated bioconcentration factors (BCFs) and bioaccumulation factors (BAFs). BAFs are measures of the bioaccumulation of substances in an organism pursuant to environmental exposures, plus exposures to the substances through food/water intake. BAFs are the ratios of tissue or plant concentrations of a substance to the concentrations that the organism is exposed to through these various routes. In comparison, BCFs consider only environmental exposures and are the ratios of the concentrations of a substance in the organism to the concentrations in the soil, water, or air to which the organism is exposed. Generally, BCFs <10, 10–50, and 50–100 indicate low, moderate, and high bioaccumulative potential, respectively (Kuperman et al., 2003a). In some of the studies examined, the terms BCF and BAF appear to be used interchangeably. This seems to be particularly true of studies examining bioconcentration in plants, in which the only, or main, source of the chemical of interest was soil. The BCF ranges above were used to evaluate the “BAFs” reported in these studies.

#### **4.4.1 Potential for Uptake from Soil and Bioconcentration in Plants**

There is sparse information on the uptake and bioconcentration of CL-20 in plants. The available information indicates that bioconcentration is minimal. In Gong et al. (2004), CL-20 was shown

to be readily taken up by ryegrass (*Lolium perenne*) grown in soil containing nominal concentrations of 0, 10, 100, 1,000, and 10,000 mg/kg CL-20. After 15–16 days of growing in the soil, the amount of CL-20 taken up by the plants was measured. The greatest concentrations of CL-20 measured in the tissue of plants grown in soil containing 9.55 and 98.4 mg CL-20/kg soil (corresponding to nominal concentrations of 10 and 100 mg/kg) were 0.21 and 9 mg CL-20/kg dry plant weight, respectively. BCFs derived by dividing the CL-20 concentrations measured in the plant tissue by the concentrations measured in the soil are 0.02 at 9.55 mg CL-20/kg and 0.09 at 98.4 mg CL-20/kg, indicating very low potential to bioconcentrate in ryegrasses.

In Rocheleau et al. (*submitted*) ryegrass was grown in sassafras loamy soil (SSL soil) or Defense Research and Development Canada sandy soil (DRDC soil) containing CL-20 for 42 days. The final concentrations of CL-20 in the soil after the 42-day exposure period ranged from 8.6 to 9,457 mg CL-20/kg SSL soil and 9.7 to 10,312 mg CL-20/kg DRDC soil. The BCFs reported for the shoots of the plants ranged from 0.01 to 0.2 for SSL soil and 0.01 to 0.5 for DRDC soil, indicating very low potential to bioconcentrate. The BCFs derived from the roots of the plants grown in soil containing the lowest final concentrations of CL-20 tested in the study (8.6 mg CL-20/kg SSL soil and 9.7 mg CL-20/kg DRDC soil) were about 12 and 20 for SSL soil and DRDC soil, respectively. The BCFs derived from the roots of the plants in soil (SSL or DRDC soil) containing 99 to 10,312 mg CL-20/kg soil ranged from 0.01 to 4.7. Thus, CL-20 appears to have, at most, a moderate potential to bioconcentrate in the roots of ryegrasses.

RDX has been shown to be taken up by plants grown in either soils or hydroponic solutions containing RDX. RDX uptake has been documented in several plant species, including wheat (*Triticum aestivum*), Blando brome (*Bromus hordeaceus*), hybrid poplars (*Populus spp*), bush beans (*Phaseolus vulgaris*), alfalfa (*Medicago sativa*) and ryegrass (Harvey et al., 1991; Cataldo et al., 1993; Yoon et al., 2006).

BCFs for RDX in ryegrass and alfalfa were determined to be 17 and 37, respectively, following a 55-day growing period in soil containing 1,540 mg RDX/kg (Best et al., 2006). In Rocheleau et al. (*submitted*) ryegrass was grown in SSL soil containing RDX for 42 days. The final concentrations of RDX in the soil after the 42-day exposure period ranged from 8.1 to 9780 mg RDX/kg soil. The BCFs reported for the shoots of the plants ranged from 0.2 to 14.7 and for the roots from 0.1 to 5.4. These values indicate moderate RDX bioconcentration.

However, continued growth in the RDX-containing soils leads to increased RDX breakdown by the plant. Additional studies support the hypothesis that RDX is broken down in plants. In Just and Schnoor (2004), reed canary grass (*Phalaris arundinacea*) was shown to facilitate the photochemical degradation of RDX. Parrotfeather (*Myriophyllum aquaticum*) and Madagascar periwinkle (*Catharanthus roseus*) were also able to break down RDX following growth in hydroponic solution containing 8 mg RDX/L for 16 days (Bhadra et al., 2001). Thus, breakdown processes are likely to partly offset the indication of a moderate bioconcentration potential provided by the BCF values.

TNT is readily taken up by *Arabidopsis thaliana* (thale cress), onion plants (unspecified species), and poplar (Kurumata et al., 2005; Kim et al., 2004; Yoon et al., 2006). Specific data on the bioconcentration of TNT in plants were not found, but *Picea abies* (Norway spruce) and *Salix spp.* (hybrid willow) have been shown to have a significant capacity to degrade TNT taken up from the soil (Schoenmuth and Pestemer, 2004).

#### 4.4.2 Potential for Bioaccumulation in Terrestrial Wildlife, Fish, and Soil Invertebrates

Toxicity studies examining the impact of CL-20 on aquatic/benthic organisms have not directly addressed bioaccumulation, and no mammalian toxicity or bioaccumulation information is available. However, in their study on the effects of CL-20 on the Japanese quail (*Coturnix coturnix japonica*), Bardai et al. (2005) attempted to extract measurable CL-20 from the heart, spleen, and brain of birds in subacute and subchronic CL-20 toxicity studies. In the subacute study, the birds were exposed to pulverized commercial feed containing CL-20 by gavage to provide a daily oral dose of up to  $5,304 \pm 53$  mg/kg bw CL-20 for the first 5 days of the study, with necropsy performed on day 14. In the subchronic study, birds were fed *ad libitum* a diet containing up to  $1,085 \pm 52$  mg CL-20/kg feed for 42 days, with necropsy immediately following the exposure period. Organs spiked with concentrations of CL-20 ranging from approximately 0.1–1.8 µg CL-20/g dry weight were used as controls. Although recoveries ranging from 99–105 percent were obtained from the spiked samples, no CL-20 was detected in any of the organs of the treated birds. This finding indicates that CL-20 is unlikely to bioaccumulate in *C. japonica*.

There is a limited amount of information on the bioaccumulation of RDX and TNT in wildlife, aquatic organisms, and soil invertebrates. RDX was found not to be bioaccumulative in deer tissue at exposure concentrations expected in the environment (ATSDR, 1996). BCFs for the earthworm (*Eisenia fetida*) ranged from 45–79 for RDX at a measured concentration of 87 mg RDX/kg soil (Kuperman, 2003a). However, at a higher soil concentration (985 mg/kg), the BCF was lower (3.5–6.8), indicating minimal bioaccumulative potential (Kuperman, 2003b). BAFs for RDX in bluegill (*Lepomis macrochirus*), channel catfish (*Ictalurus punctatus*), and *Pimephales promelas* (fathead minnow) were 1.9–6.4, 1.2–5.5, and 1.4–5.9, respectively (U.S. Army, 1984). These values are all well below what would be expected of a notably bioaccumulative substance. The BAF in fathead minnows fed *Lumbriculus variegatus* worms contaminated with TNT was reported to be 0.018 (Houston and Lofufo, 2005). Thus, TNT appears to have even less potential than RDX to bioaccumulate in aquatic species.

### 4.5 Toxicity of CL-20, RDX and TNT

#### 4.5.1 Toxicity to Humans

To date, there are no data on the toxicity of CL-20 in humans. There is also a lack of CL-20 mammalian toxicity data. Furthermore, among chemicals for which there is toxicity data, there is none with sufficient structural similarity to CL-20 to support an extrapolation for human risk.

For RDX, accidental ingestion in humans has been associated with convulsions, muscular twitching, hyperactive reflexes, headaches, nausea and vomiting, and memory loss (Stone et al., 1969). No fatalities have been reported as a result of RDX ingestion, and recovery has generally been complete within 1–2 months (Stone et al., 1969). The reference dose (RfD) for RDX has been estimated to be 0.003 mg/kg/day for oral exposure (U.S. EPA, 2006; value last revised in 1993), based on inflammation of the prostate observed in a two-year rat feeding study (U.S. DoD, 1983a). The RfD represents an estimate of the daily oral exposure to a human population (including sensitive subpopulations) likely to be without appreciable risk of adverse effects during a lifetime.

ATSDR (1996) has reported that personnel exposed to high concentrations of TNT during TNT production experienced adverse health effects, including anemia and abnormal liver function.

The oral RfD for TNT is 0.0005 mg/kg/day (U.S. EPA, 2006), based on adverse liver effects seen in a 26-week dog feeding study (U.S. DoD, 1983b).

For both RDX and TNT, the RfDs are relatively low. However, these values are very conservatively set, largely because of the uncertainty associated with the extrapolation of the results of animal studies to humans and the limited amount of data available.

#### **4.5.2 Toxicity to Environmental Receptors**

##### **4.5.2.1 Toxicity of CL-20 to Plants**

Gong et al. (2004) determined the toxicity of CL-20 to ryegrass (*L. perenne*) and alfalfa (*M. sativa*), representing monocotyledon and dicotyledon plants, respectively. Seeds were sown in Sassafras Sandy Loam soil (SSL: 0.3 percent organic carbon; 11 percent clay; pH 5.0) and GS-3 soil (3.5 percent organic carbon; 30 percent clay; pH 6.5) to which various concentrations of CL-20 were added. After 5 days for alfalfa and 7 days for ryegrass, the soil was examined for newly emerged seedlings. The seedlings were grown for another two weeks until the study was terminated. No concentration-dependent adverse effects were observed in either plant species up to a nominal concentration of 10,000 mg CL-20/kg in either soil type.

Rocheleau et al. (*submitted*) report lowest observed adverse effects concentrations (LOAECs) >9,604 mg CL-20/kg soil for shoot growth and 9,604 mg CL-20/kg soil for root growth in ryegrass grown for 21 days in SSL or DRDC soil. In comparison, the LOAEC was >8,867 mg RDX/kg soil for both shoot growth and root growth in this study.

Other studies on RDX indicate that it is likely to be more toxic than CL-20 to plants. Winfield et al. (2004) conducted a thorough investigation of potentially adverse effects using 15 plant species representing both monocotyledons and dicotyledons. Following a 6-week growing period in contaminated soil, necrotic spots and curled leaf margins were observed in some plants at concentrations as low as 5.8 mg RDX/kg in young sensitive plants. Sunflower plants (*Helianthus annuus* L.) and dicotyledons in general were found to be particularly sensitive to RDX exposure (Winfield et al., 2004). In contrast, Best et al. (2006) reported no significant reduction in the biomass of *L. perenne* and *M. sativa* after 55 days in up to 1,540 mg RDX/kg soil.

Some plant toxicity data are available for TNT. For example, EC<sub>20</sub>s for the growth of alfalfa, Japanese millet, and ryegrass shoots ranged from 43–61 mg TNT/kg soil following 13 weeks of exposure to TNT freshly amended in SSL soil (Rocheleau et al., 2006). TNT was found to have adverse effects on the emergence and biomass of lettuce (*Lactuca sativa*) and barley (*Hordeum vulgare*) when grown in silica and forest soils (Robidoux et al., 2003). Adverse effects were more marked in silica soils. *H. vulgare* growth was decreased at soil concentrations of  $55.9 \pm 4.5$  mg RDX/kg in silica soils and  $291.9 \pm 42.8$  mg RDX/kg in forest soils (Robidoux et al., 2003). Thus, the available toxicity data indicates that TNT, like RDX, is likely to be more toxic than CL-20 to plants.

##### **4.5.2.2 Toxicity of CL-20 to Soil Invertebrates and Microbes**

The impact of CL-20 on soil invertebrates has been addressed in a number of studies, as these organisms are among the most likely to be exposed to CL-20. The toxicity data available for these organisms will likely serve as the basis for developing ecological-risk-screening concentrations for CL-20 in the future. In Robidoux et al. (2004), the toxicity of CL-20 to the earthworm (*Eisenia*



*andrei*) was determined in two natural soils: SSL soil and a natural sandy forest soil (RacFor2002: 20 percent organic carbon; pH 7.2). Following 28 days of exposure, CL-20 was found not to be lethal up to concentrations of 125 mg/kg (the highest concentration tested) in RacFor2002 soil. However, in SSL soil, *E. andrei* lethality was observed at 90.7 mg CL-20/kg, and the median lethal concentration (LC<sub>50</sub>) was 53.4 mg/kg. After 56 days of exposure, the impact of CL-20 on reproductive indicators was assessed (Robidoux et al., 2004). The number of *E. andrei* juveniles was decreased at  $\geq 0.2$  mg CL-20/kg in SSL soil and at  $\geq 1.6$  mg CL-20/kg in RacFor2002 soil. Additionally, CL-20 reduced the total and hatched numbers of cocoons in both SSL and RacFor2002 soil. The EC<sub>20</sub> for both a reduction in the total number of cocoons and a reduction in hatched cocoons was  $<0.02$  mg/kg in SSL soil. In RacFor2002, the EC<sub>20</sub> for the reduction in cocoon numbers was 0.62 mg/kg, and the EC<sub>20</sub> for the reduction of hatched cocoons was 0.67 mg/kg. Therefore, reproductive toxicity was observed in both types of soil at relatively low concentrations. For all toxicity screens, greater toxicity was observed in SSL, probably because of the lower percent organic carbon and consequently lower adsorption of CL-20 and its greater bioavailability.

Similar toxicity screens were conducted for the potworm, *Enchytraeus crypticus*, as described by Kuperman et al. (2006b). In this study, *E. crypticus* adult survival and juvenile production was measured in after exposure to CL-20 freshly amended or weathered-and-aged in SSL soil. The data are summarized in Table 4-6.

Based on these data, survival and reproduction of the potworm, like the earthworm, were adversely affected by CL-20 at relatively low soil concentrations. The adverse effects appear to be slightly more marked with CL-20 weathered-and-aged in soil. This suggests that a breakdown product or products might be responsible for the toxicity observed in these studies.

**Table 4-6. Summary of CL-20 Toxicity to *Enchytraeus crypticus* in Freshly Amended and Weathered/Aged SSL Soil\***

Type of Exposure	Adult survival toxicity values (mg CL-20/kg dry soil)				Juvenile production (mg CL-20/kg dry soil)			
	NOEC	LOEC	EC <sub>20</sub>	EC <sub>50</sub>	NOEC	LOEC	EC <sub>20</sub>	EC <sub>50</sub>
Freshly amended	5 ( <i>p</i> =0.068)	10 ( <i>p</i> =0.003)	6 ± 4	18 ± 15.5	0.11 ( <i>p</i> =0.209)	0.27 ( <i>p</i> <0.0001)	0.1 ± 0.035	0.3 ± 0.1
Weathered and aged	3.1 ( <i>p</i> =0.055)	6.8 ( <i>p</i> =0.006)	>6.8	>6.8	<0.06	0.06 ( <i>p</i> <0.0001)	0.035 ± 0.01	0.1 ± 0.035

\* Adapted from Kuperman et al., 2006b.

NOEC = No observed effect concentration

LOEC = Lowest observed effect concentration

EC<sub>20</sub> = 20% effective concentration

EC<sub>50</sub> = 50% effective concentration

Dodard et al. (2005) determined LC<sub>20</sub>s and LC<sub>50</sub>s for *E. crypticus* and *Enchytraeus albidus* (another species of potworm) in three types of soil: SSL, RacAg2002, and a composite agricultural-forest soil (Rac50-50). Rac50-50 is composed of 23 percent organic matter and 2 percent clay, and has a pH of 7.9. In almost all cases, the LC<sub>20</sub>s and LC<sub>50</sub>s were below 1.0 mg CL-20/kg. The exceptions were the LC<sub>20</sub> and LC<sub>50</sub> for *E. albidus* in RacAg2002, for which the values were expressed simply as >1.0 mg/kg. However, juvenile EC<sub>20</sub>s and EC<sub>50</sub>s for *E.*

*crypticus* in all three types of soils, and *E. albidus* in Rac50-50 were even lower, and in all cases were less than 1.0 mg/kg.

The toxicity of CL-20 has been directly compared to those of the energetic compounds HMX and RDX. Among the three MCs, CL-20 is considerably more toxic to soil invertebrates than HMX and RDX. The results summarized in Tables 4-7 and 4-8 show that no observed effect concentrations (NOECs) and lowest observed effect concentrations (LOECs) for adult survival and juvenile production are considerably lower for CL-20 than for HMX and RDX. Dodard et al. (2005) reported no statistically significant decrease in adult *E. albidus* or *E. crypticus* survival up to measured concentrations of 658 mg RDX/kg and 918 mg HMX/kg of soil. No impact on the number of *E. albidus* juveniles was seen at concentrations  $\leq 174$  mg RDX/kg, and no decrease was seen up to 918 mg HMX/kg. No decrease in the number of *E. crypticus* juveniles was seen at concentrations up to 658 mg RDX/kg or 918 mg HMX/kg soil. Thus, CL-20 is clearly considerably more toxic to soil invertebrates than either RDX or HMX.

**Table 4-7. Comparative RDX, HMX, and CL-20 Adult *Enchytraeus albidus* and *Enchytraeus crypticus* Survival Data in Rac50-50 Soil\***

Explosive Chemical	<i>E. albidus</i>		<i>E. crypticus</i>	
	NOEC (mg/kg)	LOEC (mg/kg)	NOEC (mg/kg)	LOEC (mg/kg)
CL-20	0.1	0.5	0.1	0.5
RDX	$\geq 658$	NA	$\geq 658$	NA
HMX	$\geq 918$	NA	$\geq 918$	NA

\*Data presented is described in Dodard et al. (2005).

**Table 4-8. Comparative RDX, HMX, and CL-20 Juvenile *Enchytraeus albidus* and *Enchytraeus crypticus* Reproduction Data in Rac50-50 Soil\***

Explosive Chemical	<i>E. albidus</i>		<i>E. crypticus</i>	
	NOEC (mg/kg)	LOEC (mg/kg)	NOEC (mg/kg)	LOEC (mg/kg)
CL-20	0.1	0.5	0.01	0.05
RDX	174	209	$\geq 658$	NA
HMX	$\geq 918$	NA	$\geq 918$	NA

\*Data presented is described in Dodard et al. (2005).

Kuperman et al. (2006a) report EC<sub>20</sub>s and EC<sub>50</sub>s for reproductive endpoints in three species of soil invertebrates (*Eisenia fetida*, *Enchytraeus crypticus*, and *Folsomia candida*) using CL-20, RDX or HMX either freshly amended or weathered-and-aged in SSL soil in laboratory test protocols. The ranges of these values across the species and exposure types (freshly amended and weathered-and-aged) tested were:

- 0.04 to >63 mg CL-20/kg SSL soil
- 1.6 to 142,356 mg RDX/kg soil
- 0.4 to >21,750 mg HMX/kg soil

Kuperman et al. (2006a) also report the results of studies performed using a microcosm method to assess the effects of CL-20 on litter decomposition and the indigenous soil microinvertebrate

community in SSL soil. Soil biotic activity, which controls the rate of litter decomposition, was either unaffected or stimulated in soil containing initial concentrations of CL-20 up to (and including) 10,300 mg CL-20/kg soil (8,238 mg CL-20/kg soil after 8 months). In addition, the overall composition of the microarthropod community was not affected by these concentrations of CL-20, based on the number of taxonomic groups present in the soil after 12 weeks of exposure. The effects of CL-20 on soil microarthropods and predatory nematodes in the microcosm assay were consistent with the results of standardized single-species toxicity tests of CL-20 using *Eisenia fetida* (earthworms), *Enchytraeus crypticus* (potworms), and *Folsomia candida* in SSL soil. Overall, these results provide strong support for the conclusion that CL-20 can be much more toxic to soil invertebrates than HMX and RDX.

CL-20's impact on soil microbes has also been investigated. Because SSL soil has been shown to have very low microbial activity, as measured by dehydrogenase activity (DHA) and potential nitrification activity (PNA), the effects of CL-20 on DHA and PNA in GS-3 soil were studied (Gong et al., 2004). Results indicated that CL-20 did not decrease microbial activity; it actually increased microbial activity at a nominal concentration of 10,000 mg/kg in the soil (Gong et al., 2004). This is probably because CL-20 is used as a nitrogen source by soil microorganisms.

#### **4.5.2.3 Terrestrial Wildlife**

##### **Toxicity to Mammals**

There are no toxicological data available for the effects of CL-20 in mammals.

The most prevalent adverse effects of RDX in mammals are prostate inflammation, hepatotoxicity, and central nervous system (CNS) disruption. In a two-year feeding study in rats, the lowest observed adverse effect level (LOAEL) was determined to be 1.5 mg/kg/day, based on prostate inflammation. The no observed effect level (NOEL) was 0.3 mg/kg/day (U.S. DoD, 1983a). Sub-chronic and chronic feeding studies in rodents indicated that RDX ingestion was associated with anemia, convulsions, and tremors. In rhesus monkeys, daily oral doses ranging from 0.1–10 mg/kg/day were administered for 13 weeks. All treatment regimens were associated with various signs of CNS toxicity, with clonic convulsions occurring at the highest doses (Litton Bionetics, 1974).

The LD<sub>50</sub> of TNT in mice is 660 mg/kg (Dilley et al., 1982). Subchronic and chronic exposures to TNT are associated with anemia and hemosiderosis in rats and dogs (Levine et al., 1984; 1990). In a two-year rat feeding study, TNT was mixed into the diet that provided 0.4, 2, 10, and 50 mg/kg/day, respectively, of TNT. The no observed adverse effect level (NOAEL) was estimated to be 0.4 mg/kg/day (U.S. DoD, 1984). In 1974, the DoD conducted a 90-day toxicity study in beagles administered TNT in the diet to provide 0.02, 0.1 and 1.0 mg/kg/day, respectively. A slight increase in hemosiderosis of the bone marrow in the 1 mg/kg/day group was observed. The small number of animals used in this study precluded the determination of a NOAEL or LOAEL. In another study conducted by the U.S. DoD in 1978, Swiss-Webster mice, Sprague-Dawley rats, and beagle dogs were treated with TNT in the diet. The dogs were the most sensitive species tested, exhibiting a NOAEL of 0.2 mg/kg/day and a LOAEL of 2.0 mg/kg/day.

##### **Toxicity to Birds**

A study by Bardai et al. (2005) investigated the effects of dietary administration of CL-20 in Japanese quail (*Coturnix coturnix japonica*). Pulverized commercial feed containing CL-20 was given by daily gavage to groups of 7–8 birds in two studies: a subacute study in which 15-day

old juvenile birds were dosed for 5 days, with blood samples taken before administration, as well as 10 and 14 days after; and a subchronic study in which 56-day old birds were fed feed containing CL-20 *ad libitum* for 42 days, with blood samples taken before sacrifice at the end of the study. For the subchronic study, the embryos of treated females were also examined. Three females were housed with one male before the study, and the collected eggs incubated and examined to verify fertility. Throughout the study, a subset of the eggs (~10–12) were placed at 16°C for 5 days, incubated at 37.8°C for 8 days, and then cooled to 4°C before removing and weighing the embryos. In both studies, birds were monitored daily for changes in health, body weight, and feed consumption. Upon study completion, the quail were euthanized, and the authors analyzed selected tissues to measure CL-20 concentrations.

In the subacute study, birds receiving daily gavages of 307, 964, 2,439, 3,475, and 5,304 mg/kg bw CL-20, respectively, in feed for the first 5 days of the study were evaluated for toxic effects until study termination at 14 days, when full necropsies were conducted. None of these dose groups demonstrated overt signs of toxicity. There was a decrease in average weight gain in the 2,439 mg/kg and higher dose groups, but this effect was limited to the first few days of the study and was not detected 10 or 15 days after the start of the dosing schedule. Additionally, plasma sodium and creatinine concentrations were increased, and the liver-to-body-weight ratios were increased at the end of the study in birds treated with 5,304 mg CL-20/kg bw/day.

In the subchronic study, 11, 114, or 1,085 mg CL-20/kg feed was provided *ad libitum* to the respective groups for 42 days. Plasma biochemical parameters were assessed following the treatment period. An increase in aspartate aminotransferase was observed in the 1,085 mg CL-20/kg feed group. Throughout this study, no differences in feed consumption or body weight were observed among exposure groups. Thus, both studies demonstrated that CL-20, *per os*, does not adversely affect adult birds even at relatively high doses.

However, CL-20 was found to adversely impact quail embryo weights, beginning with the group of embryos born of females treated with 11 mg CL-20/kg. The number of eggs produced by females in each group did not differ significantly, and no developmental delays were associated with CL-20 treatment. The malformation results were difficult to interpret because a large number of embryos were inadvertently dehydrated in a manner that made them unsuitable for the study. Of the few embryos that were not dehydrated, Bardai et al. (2005) reported that (1) 2/6 embryos in the 114 mg CL-20/kg group had multiple cranial and facial deformities, and (2) 3/9 embryos in the highest dose group (1,085 mg CL-20/kg feed) had beak curvatures, possible mid-brain enlargement, and one-sided development with microphthalmia. None of the embryos in the control group exhibited the effects observed in the 114 mg/kg or 1,085 mg/kg treatment groups, but 2/9 control embryos showed very slight ocular asymmetric deviations. This study suggests that although CL-20 causes minimal toxicity in adult birds, it may adversely impact avian development. Further studies will be needed to confirm that there is any developmental toxicity attributable to CL-20 exposure.

In comparison, RDX causes CNS disturbances in the northern bobwhite (*Colinus virginianus*), and is lethal to that bird at a single oral dose  $\geq 187$  mg/kg bw (Gogal et al., 2003). RDX exposure was also associated with a decreased liver-to-body weight ratio and an increase in packed cell volume. Additionally, RDX contributed to an increase in heterophil counts and the heterophil-to-lymphocyte ratio, a marker of poor general avian health (Huff et al., 2005).

Gogal et al. (2002) evaluated the effects of TNT on the Northern Bobwhite (*Colinus virginianus*). Birds were treated for 90 days with TNT ranging from 100–3000 mg/kg in commercial feed. A LOAEL of 178 mg/kg/day was estimated based on mortality and abnormal histopathology (Gogal et al., 2002). The toxicity of TNT was also evaluated using the common pigeon (*Columbia livia*), following a 60-day regimen in which animals were treated via daily oral gavage (Johnson et al., 2005). Signs of toxicity were observed after two to three weeks of exposure and included weight loss, vomiting, neuromuscular effects, and scant red feces. TNT was lethal to 8/12 male and 2/12 female pigeons at the daily dose of 200 mg/kg, and lethal to 2/12 female pigeons at the daily dose of 120 mg/kg. Other dose-related outcomes were altered organ weights and changes in plasma albumin and sodium concentrations (Johnson et al., 2005).

### **Toxicity to Amphibians**

No amphibian toxicity data were available for CL-20.

A study in which groups of red-backed salamander (*Plethodon cinereus*) were exposed to 0, 10, 100, 1000, and 5,000 mg RDX/kg soil for 28 days resulted in signs of neuromuscular effects, including lethargy, gaping and tremors, and also significant weight loss in the highest concentration group (Johnson et al., 2004). In a second study investigating the impact of TNT on tiger salamanders (*Ambystoma tigrinum*), the salamanders were exposed to TNT in a soil matrix and fed earthworms that had been previously exposed to TNT in the soil for 14 days. At the start of the study, the soil concentration was 280 mg TNT/kg; at the end of the study, the soil concentration was 59 mg TNT/kg. The concentrations of TNT in the earthworms ranged from 0.25–0.62 mg/kg. No adverse effects were noted in any of the salamanders (Johnson et al., 2000).

Using the African clawed frog (*Xenopus laevis*) teratogenesis assay (FETAX), Saka (2004) reported that the 96-hour LC<sub>50</sub> for TNT was 3.8 mg/L and the EC<sub>50</sub> for developmental effects was 2.2 mg/L. Axial malformations and eye abnormalities were common.

### **Toxicity to Reptiles**

No reptile toxicity data were located for CL-20, TNT, or RDX.

#### **4.5.2.4 Toxicity to Aquatic/Benthic Organisms**

The toxicity of CL-20 was determined in freshwater algae (*Selenastrum capricornutum*) and in the Microtox test (using the luminescent bacteria *Vibrio fischeri*). The goal of the Microtox test is to assess toxicity by determining effects on cellular respiration. A reduction in the luminescence of the test bacteria indicates a decrease in cell respiration.

For both assays, CL-20 was dissolved in acetone and then diluted in water to achieve 1 percent v/v acetone in water for each CL-20 concentration. This concentration of vehicle had previously been shown not to be toxic to the test species. The highest CL-20 concentration tested was the solubility limit,  $3.59 \pm 0.74$  mg/L at 25°C (Gong et al., 2004). This concentration had no impact on either *V. fischeri* or *S. capricornutum*. In contrast, the IC<sub>50</sub> for TNT in *V. fischeri* was 0.27–0.94 mg/L and the IC<sub>50</sub> for *S. capricornutum* was 0.62–1.14 mg/L (Sunahara et al., 1999).

Results of aquatic toxicity tests with CL-20 indicated IC<sub>20</sub>s of 2.0 mg/L for fathead minnow (*P. promelas*) growth and 1.2 mg/L for water flea (*C. dubia*) survival and reproduction (Kuperman et al., 2006a). Preliminary results reported for CL-20 by Haley et al. (2003) suggest an IC<sub>20</sub> of 13 mg/L for the growth of green single-celled algae (*S. capricornutum*). These results indicate that CL-20 can have considerable toxicity to aquatic organisms.

The toxicity of TNT and RDX to the estuarine amphipod *Eohaustorius estuarius* was evaluated by adding the chemicals to the sediment in two separate aquatic environments for ten consecutive days (Rosen and Lotufo, 2005). For RDX, no mortality was seen up to the highest measured sediment concentration of 2,400 mg/kg during the ten-day period. TNT was considerably more toxic; LC<sub>50</sub>s for *E. estuarius* in the two environments were 35 mg TNT/kg and 2.8 mg TNT/kg, respectively. The 96-hour LC<sub>50</sub>s for RDX in zebrafish (*Danio rerio*) were 22.98 and 25.64 mg/L in two separate trials. For these same trials, the NOECs were  $13.27 \pm 0.05$  and  $13.32 \pm 0.30$  mg/L, and LOECs were  $16.52 \pm 0.05$  and  $19.09 \pm 0.23$  mg/L in several trials (Mukhi et al., 2005). Thus, both TNT and RDX are likely to be less toxic to aquatic organisms than CL-20, though additional studies are needed to confirm this preliminary conclusion.

## **5 Relative Risk Characterization**

### **5.1 Human Health Risk**

The impact of CL-20 on human health cannot be reliably determined from the existing data. Data pertaining to human—or at least mammalian—CL-20 toxicity are needed to enable the comparative evaluation of the risks of CL-20 to human health relative to other explosive MCs.

### **5.2 Environmental Receptors**

From the available data on a single plant species (ryegrass), CL-20 is apparently not notably toxic or bioaccumulative and is likely to pose less threat to terrestrial plants than RDX and TNT. In contrast, the more complete data set for soil invertebrates indicates that CL-20 is considerably more toxic to earthworm and potworm species than RDX and HMX. CL-20 may also be at least as toxic to aquatic species as RDX and TNT, although the information is inadequate to draw any definitive conclusions.

Based on a single study in the Japanese quail, CL-20 is apparently less toxic to avian species than RDX and TNT. This was also the only CL-20 study addressing possible bioaccumulation in wildlife, and no bioaccumulation was noted. No toxicity information was found for CL-20 in mammals, amphibians, or reptiles.

### **5.3 Uncertainty Assessment**

There are critical uncertainties in virtually every key information area that needs to be addressed completely in a comprehensive, technically defensible relative risk characterization of CL-20 and RDX. There are exceptions:

- CL-20 will degrade to produce many endproducts in common with RDX.
- CL-20 is clearly and substantially more toxic to soil invertebrates than RDX.
- CL-20 is clearly toxic to aquatic microorganisms, invertebrates, and animal species.
- CL-20 is clearly and substantially less toxic than RDX to adults of a single bird species tested.

However, the certainties represented by these four exceptions are insignificant compared with the overall uncertainty associated with the other key information areas.

First, there are no human, mammalian, amphibian or reptilian toxicity data for CL-20. The lack of any such data precludes both a human health and a terrestrial wildlife ecological relative risk evaluation of CL-20 and RDX. As noted above, there are data indicating that CL-20 is less toxic than RDX to the adults of one bird species tested. However, CL-20 might affect the development of this species at lower exposures than does RDX, although these results are equivocal and require further investigation. Further, the toxicity of CL-20 has not been studied in any other bird species. Thus, the CL-20 toxicity data available from avian studies cannot support an evaluation of the relative risks of CL-20 and RDX even for terrestrial avian species.

Second, toxicity data on CL-20 are available for only a few terrestrial plant species, and bioconcentration data are available for only one species. Thus, it is uncertain that the relatively low toxicity and bioconcentration potential observed in these species can be extrapolated to other plant species. The toxicity and bioaccumulation of RDX has been determined in several plant species, and the results are more certain for this constituent. However, CL-20 and RDX toxicity

have never been tested in the same plant species, adding to the uncertainty associated with the relative risks of these constituents to plants.

Third, although CL-20 clearly exhibited toxicity at least as great as that of RDX to aquatic species, the data are not sufficient to indicate whether—and if so, to what extent—CL-20 may be more toxic than RDX to these species.

Fourth, the residue produced by the thermal degradation of CL-20 is unknown, thus its potential threat to human health or the environment, if any, is also unknown.

Fifth, although the environmental degradation of CL-20 and RDX produce virtually the same breakdown end products, there is an exception. The environmental degradation of CL-20 can produce glyoxal as an end product rather than the formaldehyde that can be produced from RDX. This difference introduces an additional element of uncertainty in the assessment.



## **6 Conclusions/Recommendations**

### **6.1 Regulations**

Regulatory standards and guidelines are usually developed by regulatory agencies and other organizations to address substantial, widespread, or persistent environmental contamination on a regional or national scale. Thus, unless CL-20 usage on training ranges is substantially greater than currently expected or unless substantial testing of CL-20–based munitions occurs at more than just a few test ranges, there is limited likelihood that such standards and guidelines will be developed for CL-20. If, however, such standards and guidelines are developed for CL-20 in the future, they could be comparable to those already established for RDX and TNT. However, the toxicity information available for CL-20 is so limited that any predictions about standards and guidelines are highly speculative.

### **6.2 Fate and Transport**

CL-20 is expected to be highly labile in the environment. The highly strained, multiply-nitrated ring structure can reasonably be expected to degrade rapidly in the environment and produce essentially the same environmental degradation end products.

The environmental degradation end products of CL-20 are essentially identical to those of RDX. The sole exception is that CL-20 degradation may yield glyoxal rather than formaldehyde produced from RDX.

The evidence reported in Table 3-5 indicates that the thermal degradation products of CL-20 are also thermal degradation products of RDX, except that CL-20 may also yield gaseous isocyanic acid—which can be expected to dissipate rapidly in the air after an explosion—and a poorly characterized solid residue. There is no information available to indicate whether this residue might pose a threat to human health or the environment.

All of the energetic chemicals examined in this report, including CL-20, exhibit very low water solubilities. In addition, there generally appear to be no substantial differences in other environmentally-relevant physicochemical properties of CL-20 and RDX (e.g.,  $K_d$ ,  $K_{oc}$  and vapor pressure).

One potentially differentiating characteristic is that, unlike RDX and HMX, CL-20 tends to sorb to organic matter in environmental matrices rather than to the inorganic material in them. Thus, there may be a greater tendency for CL-20 to be retained in matrices containing higher proportions of organic matter (e.g., in the surface soils of a tropical environment). However, even this difference between CL-20 and RDX (and HMX) appears to be too small to be significant.

Generally, the results of the available studies and the examination of the pertinent parameters indicate that the fate and transport of CL-20 in the environment will not differ substantially from that of RDX.

### **6.3 Toxicology**

There are no human studies or anecdotal reports of accidental exposures available to evaluate the potential toxicity of CL-20 to humans. Further, there are no toxicity studies available on mammalian test species that would support predicting the effects and risks of CL-20 in humans. In addition, no toxicity studies exist for structurally closely related compounds. Thus, none of them can serve as

surrogates for the estimation of the risks to human health associated with potential exposures to CL-20 or to provide a comparative evaluation of risks associated with CL-20 and RDX.

The results of studies on the environmental degradation of CL-20 and RDX indicate that CL-20, unlike RDX, may yield significant quantities of glyoxal as an end product in soil and water. RDX degrades in the environment to produce formaldehyde rather than glyoxal.

Both glyoxal and formaldehyde would be expected to mineralize rapidly in moist soils and aqueous environments.

No toxicity studies have yet been conducted on amphibian and reptile species.

Studies on plants indicate that CL-20 is unlikely to be toxic to plants or to bioconcentrate in plant species. Similarly, RDX and TNT do not appear to bioconcentrate in plants. However, unlike CL-20, both RDX and TNT in soil have been reported to produce toxic effects in plant species. Thus, CL-20 might be considered to pose less threat to plant life than RDX or TNT.

Toxicity studies on soil invertebrates, aquatic species, and birds are available for CL-20, RDX, and TNT. These studies reveal that CL-20 may be more toxic to soil invertebrates, at least as toxic to aquatic species, and less toxic to birds than RDX and TNT. Further, CL-20 did not appear to bioaccumulate in the bird species tested, unlike RDX and TNT, which exhibit a tendency to bioaccumulate.

The observation that CL-20 may be more toxic to soil invertebrates than RDX is significant, because the measured toxicity of a compound to soil invertebrates often serves as the basis for deriving ecological-risk-screening values. However, an important characteristic of these values is that they are generally considered to be highly conservative threshold concentrations used for the preliminary evaluation of soil contaminant concentrations at a site. Exceeding such ecological-risk-screening concentrations can indicate that a more advanced, site-specific ecological risk assessment may be warranted for a site. This may include a comprehensive evaluation of the potential for the contaminant to bioaccumulate in the food chain and to adversely affect species at the higher trophic levels found at the site. However, comparing an ecological-risk-screening concentration to site concentrations cannot serve as a credible or technically defensible basis for deciding to remediate a site.

Accordingly, the greater toxicity of CL-20 to soil invertebrates observed in the available studies cannot be used to predict greater risks to the environment compared with RDX. This is especially true because CL-20 has also been shown to be less toxic to birds, which can presumably represent at least some of the higher trophic level species that may be present at a site. On the contrary, the overall results suggest that the environmental risks associated with CL-20 will be less than those of RDX for terrestrial species. However, the available information is not adequate to draw this conclusion either.

The observation that CL-20 is at least as toxic, and may be more toxic, to aquatic organisms as RDX and TNT is also insufficient to indicate whether CL-20 may be substantially more toxic to these organisms than RDX or TNT. Again, the information is inadequate to conclude that CL-20 may pose a greater threat to aquatic environments than the other energetic chemicals tested.

## **6.4 Relative Risk Assessment**

The results of the studies and factors reviewed in this report indicate that the current information is not sufficient to determine whether CL-20 will likely represent a greater or lesser threat to human health or the environment than RDX. It may pose a lower threat if it is used in much smaller quantities on ranges than RDX.

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