Development of a Relative Source Contribution Factor for Drinking Water Criteria: The case of Hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX)

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Abstract

In protecting human health, the application of fate, transport, and exposure data are essential in the development of chemical-specific criteria for drinking water. There are few environmental regulations, standards, or guidance values for hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX or Royal Demolition eXplosive), but an increasing number of states are developing standards and guidelines for RDX. RDX is a synthetic chemical, which is not known to occur naturally. It is a military munitions explosive and has limited civilian uses. Available data suggest that RDX is not anticipated to be a national exposure concern. This assessment presents the development of a relative source contribution (RSC) factor for RDX. An RSC accounts for all sources and non-occupational exposures from RDX and apportions these amounts to each source so that an individual's total dose does not exceed the reference dose (RfD). The application of the Exposure Decision Tree approach (subtraction method), recommended by the US Environmental Protection Agency (USEPA), was used to determine the RSC. A hypothetical exposure model was utilized that identified the relevant potential sources for highly exposed receptors proximate to an area where RDX was released. Potentially contaminated media include soil, groundwater, and surface water. Potential exposure pathways include ingestion of soil, water, and contaminated local crops and fish; dermal contact with soil; and from water used in bathing. These pathways are not applicable nationally, but are limited to areas that are in close proximity to current or former military bases where RDX may have been released into the environment. Given the physical/chemical properties and the available environmental occurrence data on RDX (from current or former military sites), there are adequate data to support a chemical-specific RSC term for RDX of 50 percent for drinking water ingestion. (The opinions herein are those of authors and do not necessarily reflect the opinions of the USEPA or the Department of the Army).

Background

Hexahydro-1, 3, 5-trinitro-1, 3, 5-triazine (RDX), is a synthetic chemical used as an explosive in both military and civilian applications. It can be released into the environment (primarily water and soil) during manufacturing and disposal, and from military training operations. RDX is slightly soluble in water, but it has been detected in both groundwater and surface water at or near Army Ammunitions Plants (AAP) that manufacture the chemical or assemble munitions containing the explosive (Talmage et al., 1999). The potential of RDX to be found in soils and groundwater at sites of munitions production, testing, or disposal raises concerns over the potential bioavailability from soils, surface and ground waters from sites contaminated with RDX. Several studies have indicated that RDX is rapidly assimilated by the roots of higher plants (trees) and by forage and crop plants from soils (Cataldo et al., 1990; Fellows et al., 1995; Checkai and Simini, 1996; Checkai et al., 1996; Price et al., 1997) and nutrient solutions (Cataldo et al., 1990; Harvey et al., 1991; Price et al., 1997). Given that human exposure of RDX may occur through contact with contaminated environmental media, the Department of Defense (DoD) is leading an effort to evaluate information on RDX exposures and human health risk. This information is used here to develop a relative source contribution (RSC) for RDX.

The USEPA calculates a RSC as part of deriving drinking water health advisories and drinking water standards. The RSC is meant to ensure that when populations are exposed to a chemical from multiple sources, the total exposure will not exceed the reference dose (RfD) (USEPA, 2000). Development of a RSC is an attempt to account for all sources and routes of non-occupational exposures. RSCs are calculated for chemicals that are non-carcinogens or threshold carcinogens. Information currently available indicates that exposure to RDX is not widespread and there are adequate data available to move from the default RSC of 20 percent recommended by the USEPA (USEPA, 2000). There may be site-specific situations where populations are living near current or former military installations that produce or use RDX containing materials and therefore may be exposed to some level of RDX. The USEPA encourages states and authorized tribes to make alternative exposure and RSC estimates based on local data. These local situations would be evaluated on a site-specific or local basis. We report here an approach that may be used to calculate a RSC with local information.

Methods and Results

A literature search was completed in mid-2007 for sources, uses, fate and transport, monitoring, toxicity, and exposure data related to RDX, including peer-reviewed literature and technical reports, using Medline (PubMed), DTIC (Defense Technical Information Center), SciFinder, and the Internet. Secondary published sources were also reviewed (e.g., ATSDR, 1995 and US EPA IRIS, 2008). Non-published reports related to the environmental investigations of Department of Defense (DoD) sites under the Defense Environmental Restoration Program were not examined. In addition, to assess additional sources of RDX to the environment we searched the Hazardous Substance Data Bank, the Household Products Database, and the USEPA Pesticide Product Information System.

The available environmental occurrence and measurement data were almost exclusively limited to military facilities associated with the manufacture of RDX, or military firing ranges where munitions containing RDX have been used (Table 1). Available data as well as chemical and physical properties (Table 2) were considered and a conceptual exposure model was developed (Figure 1). All available information (Tables 3, 4 and 5) was utilized for derivation of a relative source contribution for RDX using the USEPA Exposure Decision Tree (USEPA 2000) (Figure 2).

Although RDX concentrations in soil, sediment, groundwater, and surface water are available from a number of military installations, concentrations in the various media range widely and the data are not amenable to developing a meaningful national upper bound or central tendency estimates.

Table 1: Sources of Exposure and Uses of RDX (in the US)

Sources	Uses and Exposure
Synthetic chemical production: Limited to Holston AAP (Tennessee) - Manufactured for military explosives and used in munitions	RDX reaches environment via the waste streams
Several AAPs load and package RDX	RDX reaches environment via the waste streams
Artillery Ranges, primarily from artillery and mortar rounds	Heterogeneous contamination from what can be considered randomly distributed point sources
Disposal and Demolition of Stockpiles	

The chemical and physical properties of RDX (Table 2) do not suggest widespread dispersion in the environment; RDX has low water solubility, slow dissolution in aqueous solution, low vapor pressure, and a low affinity for hydrophobic substances, which suggests that RDX would have limited retention in soil. Nonetheless, laboratory and field studies have demonstrated RDX's potential to leach from soil— it has a medium-to-high mobility in soil resulting in its potential to leach to groundwater (McGrath 1995; Pennington et al. 1995; Cataldo et al. 1990).

Table 2: Physical and Chemical Properties of RDX

Identification	RDX	Reference*
CAS Number	121-82-4	HSDB 2009
Molecular Formula	$C_3H_6N_6O_6$	HSDB 2009
Physical and Chemical Properties		
Boiling Point (ºC)	276–280	HSDB 2009
Melting Point (ºC)	205.5	HSDB 2009
Molecular weight (g/m)	222.12	HSDB 2009
Log K_{oc}	0.84–2.2	USACHPPM 2002
Log K_{ow}	0.87	HSDB 2009
Water Solubility (mg/L at 25 ºC)	59.7	HSDB 2009
Vapor Pressure (mm Hg at ºC)	4.1×10^{-9}	HSDB 2009
Henry's Law Constant (atm-^{3}/mole)	1.2×10^{-5}	USACHPPM 2002

*HSDB = NLM's Hazardous Substances Data Bank
*USACHPPM = U.S. Army Center for Health Promotion & Preventive Medicine

Figure 1: Potential Pathways for Human Exposure: Conceptual Model

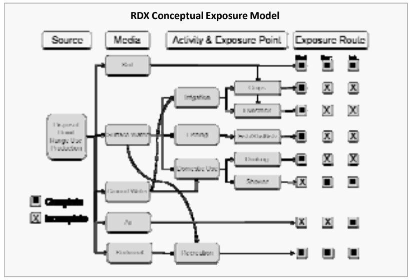

Table 3: Potential Exposure Pathways for RDX

Environmental Media	Potential Exposure Pathways
Soil	• Direct contact with the skin • Incidental ingestion of soil • Inhalation of soil particles • Ingestion of food plants grown with contaminated soils • Ingestion of livestock raised with contaminated soils*
Surface Water	• Direct contact with the skin • Ingestion of water • Inhalation contact through showering* • Dermal contact through bathing • Ingestion of fish from contaminated waters • Ingestion of food plants irrigated with contaminated water • Ingestion of livestock irrigated with contaminated water*
Ground Water	• Direct contact with the skin • Ingestion of water • Inhalation through showering* • Dermal contact through bathing • Ingestion of food plants irrigated with contaminated water • Ingestion of livestock irrigated with contaminated water*
Air	• Inhalation of particulates from incineration*
Sediment	• Direct contact with the skin during recreation activities* • Incidental ingestion of sediment during recreation activities* • Inhalation of particles during recreation activities*

* indicates those pathways that are minor sources for the general population, or otherwise not considered in quantification.

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Table 4: Summary of Environmental Measurement Data

Environmental Media	Concentration/Level	Comments
Ground water	Up to 70 mg/L.	•Detected in 11 of 34 DoD sites; two additional sites had non-detects 70 mg/L exceeds water solubility
Surface water	>0.004–109 mg/L	•Surface water bodies found only at 5 of 34 DoD sites
Soil	0.01 - 13,900 mg/kg	•Detected in 24 of 34 of Army installation sites
Sediment	2 to 120, 000 mg/kg	•Detected at five of 34 DoD sites
Drinking water	No data on RDX contamination	•Not regulated under SDWA of EPA •Being monitored under UCMR2 program (EPA 2005) •UCMR2 preliminary results - 4 detections of RDX (minimum detection level of 1 ppb) out of a total of 21,555 analyses from sampling at 3222 Public Water Systems (U.S EPA, 2010)[b]
Food	No data	
Air	No data	
Consumer products	Not applicable	

[a] Talmage et al. (1999), CHPPM (2002), etc.
[b] http://www.epa.gov/safewater/ucmr/data.html#UCMR2
DoD – US Department of Defense
UCMR2 – Second Cycle of the Unregulated Contaminant Monitoring Regulation

Data suggest that RDX can accumulate in species of field and garden crop plants that are known human foods.

Table 5: Plant Uptake (Bioconcentration) and Bioaccumulation Factors

Uptake	Bioconcentration/ bioaccumulation factors/ratios	Comments	References
Soil to plant	0.06 to 5.99	Ratios were determined in bean pod, alfalfa, tomato fruit, lettuce leaves	Cataldo et al. (1990); Price et al. (1997); Lachance et al. (2003)
Water to plant	0.16 to 5.50	Ratios were determined in tomato fruit, lettuce leaves, bush bean fruit, and radish root	Checkai and Simini (1996); Checkai et al. (1996); Price et al. (1997)
Wildlife, deer, liver, muscle	Not detected		Whaley and Leach (1994); USACHPPM (2002)
Fish	1.5 to 5.9 ml/g	Channel catfish, bluegill sunfish, fathead minnows, juvenile sheephead minnows	Bentley et al. (1977); Lotufo and Lydy (2005); Liu et al. (1983); Houston and Lotufo (2005)

Figure 2: Exposure Decision Tree for Defining Proposed and Uses of RfD (or POD/UF) Apportionment

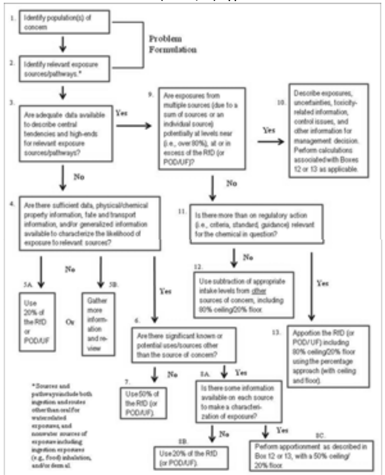

Figure 3: Exposure Decision Tree for RDX

Box 1 - Populations of Concern
RDX – General Population

Box 2 - Relevant Exposure Sources, Pathways
RDX – Figure 1

Box 3 -Adequate Exposure Data (high ends and central tendencies)?
RDX – No

Box 4 - Sufficient Data to Characterize Likelihood of Exposure?
RDX – Yes

Box 6 - Other sources or uses of RDX?
RDX – No

Box 7 – Use 50% of the RfD

Discussion and Conclusions

RDX is not widely distributed in the environment, but detected mainly in the restricted areas of near waste disposal of military manufacturing sites and at military training ranges. RDX is not a chemical regularly monitored in drinking water;, however, preliminary data under the ongoing UCMR2 program suggest that RDX is not likely to be of national concern (USEPA 2010). There are no data on RDX in market basket foods and consumer products. It is unlikely that farmers may grow crops in RDX-contaminated soils or irrigate such crops with RDX-contaminated water given that RDX is confined to areas near its use or manufacture. At closed or transferred military installation, the soils and water are remediated prior to release of the property for civilian use.

The chemical and physical properties of RDX (Table 2) predict that it will have limited retention in soil or readily leach from soil. Several studies indicate that edible portions of garden and field crops have the potential to take up RDX from contaminated soil as well as from irrigation water. These results suggest that food crops grown in RDX-contaminated soils or irrigated with RDX-contaminated water may be a source of RDX exposure. Given the physical/chemical properties, and the lack of environmental measurement data except at military sites, there is adequate support for a chemical-specific RSC term for RDX of at least 50% for drinking water, utilizing the USEPA process.

This poster demonstrates an approach that may be used to calculate RSCs in site-specific situations where national monitoring data are not available and national exposure is not anticipated, as is the case for RDX. The approach is based on the USEPA (2000) process that provides a framework to evaluate the adequacy of the available exposure data, exposure scenarios, and relevant sources of exposure (see Figure 3). The USEPA process supports development of a chemical-specific RSC term for RDX of 50 percent.

An RSC can also be derived using site-specific exposure data, if such a local exposure situation exists. In addition, a site-specific approach based on the assumption that the relevant media will be remediated to a level dictated by a Superfund-type risk assessment may also be used. An RSC could be assigned based on a consideration of clean up goals. For example, one could select specific contaminated media for remediation, such as soil and water, determine the approximate costs of remediation of both media, and then assign an RSC to each to determine the level of clean-up. RDX exposure may be apportioned at 50% RSC to each of the soil and water media, if the costs of remediation are approximately equal between these two media, or some different proportion, if the costs are different. Remediation goals for each of the two media would be calculated based upon appropriate exposure assumptions and values.

References available upon request

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