Ground Water Quality Standard for Hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX)

CASRN# 121-82-4

February 2008 NJDEP

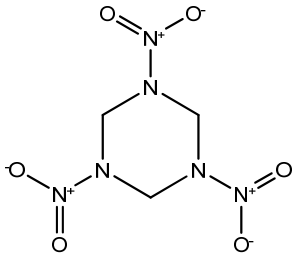
Summary of Decision: In accordance with the New Jersey Ground Water Quality Standards rules at N.J.A.C. 7:9C-1.7, the Department of Environmental Protection (Department) has developed an interim specific ground water quality criterion of 0.3 μg/L and PQL of 0.5 μg/L (ppb) for hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX). The basis for this criterion and PQL are discussed below. Pursuant to N.J.A.C. 7:9C-1.9(c), **the applicable constituent standard is 0.5 μg/L**.

hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX)

Cyclotrimethylenetrinitramine

Molecular Formula: $C_3H_6N_6O_6$

Molecular Structure:



Background: Hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX) is one of the four most important nitramine high energy explosives and is also incorporated into high performance rocket propellants. RDX has been evaluated by the U.S. Environmental Protection Agency (USEPA) and both a Reference Dose and a carcinogenicity classification (Group C, Possible Human Carcinogen) are available on the USEPA IRIS database. The Department derived a ground water quality criterion for RDX using both the USEPA IRIS Reference Dose (RfD) for a non-carcinogen, and the cancer slope factor for Group C carcinogenicity classification.

Reference Dose: The IRIS RfD for RDX is 0.003 mg/kg/day, which was developed in 1988 (USEPA, 2000) based on a two year dietary study in rats (USDOD, 1983). In this study, the most sensitive endpoint was inflammation of the prostate, which occurred at doses of 1.5 mg/kg/day and above, but was not seen at 0.3 mg/kg/day. Therefore, 0.3 mg/kg/day was considered to be the No Observed Adverse Effect Level (NOAEL). An uncertainty factor of 100, appropriate for a NOAEL from a chronic study, was applied to derive the Reference Dose of 0.003 mg/kg/day.

The IRIS cancer assessment for RDX was developed in 1990 (USEPA, 2000). An increased incidence of hepatocellular adenomas combined with carcinomas was seen in female mice in a chronic dietary study (USDOD, 1984). No statistically significant increase in tumors was seen in the male mice, nor in male or female Fischer 344 rats in a similar chronic study (USDOD, 1983). A cancer slope factor of 0.11 (mg/kg/day)-1

was derived based on the combined incidence of hepatocellular carcinomas and adenomas in female mice. For Class C chemicals, the cancer slope factor is used to develop a ground water criterion at the 10^{-6} risk level.

Derivation of Ground Water Quality Criterion: The ground water quality criterion for RDX was derived using both the 1) Reference Dose and 2) the Cancer Slope Factor, pursuant to the formula established at N.J.A.C. 7:9C-1.7(c)4.

1) Derivation based on Reference Dose: The ground water quality criterion based on the Reference Dose of 0.003 mg/kg/day (as explained above) is derived as follows, using standard default assumptions:

$$\frac{0.003 \text{ mg/kg/day} \times 70 \text{ kg} \times 0.2}{2 \text{ L/day}} = 0.021 \text{ mg/L or } 21 \text{ } \mu\text{g/L}$$

Where:
0.003 mg/kg/day = Reference Dose
70 kg = assumed body weight of average person
0.2 = Relative Source Contribution from drinking water
2 L/day = assumed daily drinking water intake

2) Derivation based on Cancer Slope Factor: The ground water quality criterion based on the cancer slope factor is derived as follows, using standard default assumptions:

$$\frac{(10^{-6} / 0.11 \text{ (mg/kg/day)}^{-1})}{2 \text{ L/day}} \times 70 \text{ kg} = 0.00032 \text{ mg/L or } 0.32 \text{ µg/L}$$

(which rounds to 0.3 µg/L)

Where:
10^{-6} = Risk Level
0.11 $(mg/kg/day)^{-1}$ = Cancer Slope Factor
70 kg = assumed body weight of average person
2 L/day = assumed daily drinking water intake

L/day = assumed daily drinking water intake

As shown above, the ground water quality criterion derived based on the cancer slope factor is 0.3 µg/l (carcinogenic end point), which is more protective than the ground water quality criterion derived based on the RfD, which is 21 µg/L (non-carcinogenic end point). Therefore, the Department has established the interim specific ground water quality criterion as 0.3 µg/L.

Derivation of PQL: The method detection limit (MDL) and the practical quantitation level (PQL) are performance measures used to estimate the limits of performance of analytic chemistry methods for measuring contaminants. The MDL is defined as "the minimum concentration of a substance that can be measured and reported with 99 percent confidence that the analyte concentration is greater than zero" (40 CFR Part 136 Appendix B). USEPA recommends that the MDL be multiplied by a factor of five or 10 to account for the variability and uncertainty that can occur at the MDL. The Department uses a value of five as the median upper boundary of the inter-laboratory MDL distribution from the New Jersey certified laboratory community and multiplies the MDL by five to derive the PQL. Establishing the PQL at a level that is five times the MDL provides a reliable quantitation level that most laboratories can be expected to meet

during day-to-day operations.

No published method was listed for RDX in the in National Environmental Methods Index (NEMI). However, TM Chow (2004) describes a trace level analysis of hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX) and its biodegradation intermediates in liquid media by solid-phase extraction and high pressure liquid chromatography analysis. The detection levels using this method were 0.1 ppb. As explained above, a more conservative detection limit is established using a multiplier of five. 0.1 ppb x 5 = 0.5 ppb. Therefore, the Department has established a PQL of 0.5 ppb for RDX.

Conclusion: Based on the information provided above (and cited below), the Department has established an interim specific ground water quality criterion of 0.3 µg/L and a PQL of 0.5 µg/L (ppb) for RDX. Pursuant to N.J.A.C. 7:9C-1.9(c), since the PQL is higher than the criterion for this constituent, **the applicable constituent standard for hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX) is 0.5 µg/L**.

Technical Support Documents: *Interim Specific Ground Water Quality Criterion Recommendation Report for Hexahydro-1,3,5-Trinitro-1,3,5-Triazine (RDX),* Dr. Gloria Post, NJDEP, December 19, 2006; *Procedure for Describing Process for Development of Analytical Practical Quantitation Levels (PQLs) for Hexahydro-1,3,5-Trinitro-1,3,5-Triazine (RDX),* R. Lee Lippincott, Ph.D, NJDEP, September 18, 2005.

References:

Chow TM, Wilcoxon MR, Piwoni MD, Adrian NR. (2004). Trace level analysis of hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX) and its biodegradation intermediates in liquid media by solid-phase extraction and high-pressure liquid chromatography analysis. J Chromatogr Sci. 2004 Oct 42(9):470-3.

USDOD (1983). U.S. Department of Defense. Available from U.S. Army Medical Research and Development Command. DAMD17-79-C-9161. Ft. Detrick, Frederick, MD 20701. (Cited in USEPA, 2000).

USEPA (2000). United States Environmental Protection Agency. Integrated Risk Information System. Hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX) (CASRN 121-82-4). Last updated 5/17/2000.