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Installation Restoration Research Program

Environmental Fate and Transport Process Descriptors for Explosives

James M. Brannon and Judith C. Pennington

May 2002

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Preface

The U.S. Army Engineer Research and Development Center (ERDC), Environmental Laboratory (EL), Vicksburg, MS, prepared this report. The research was sponsored by the Strategic Environmental Research and Development Program, Arlington, VA, Mr. Bradley P. Smith, Executive Director, and Dr. Jeff Marqusee, Technical Director, under Compliance Project Number CP1155 and the Headquarters, U. S. Army Corps of Engineers (HQUSACE), Installation Restoration Research Program (IRRP), Fate and Effects Thrust Area; the Work Area was entitled Fate and Transport of Unexploded Ordnance (UXO). Mr. Clem Myer was the IRRP Coordinator at the Directorate of Research and Development, HQUSACE. The IRRP Program Manager was Dr. M. John Cullinane, EL, ERDC.

This report was reviewed by Drs. Mark Dortch and Mansour Zakikhani, EL, ERDC. The study was conducted under the direct supervision of Dr. Richard E. Price, Chief, EPED, EL, and Dr. Edwin A. Theriot, Director, EL.

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1 Introduction

Rationale

Many U.S. Department of Army and other Department of Defense installations have soil and ground water containing elevated concentrations of explosives and energetics. Contamination by the explosives 2,4,6-trinitrotoluene (TNT), hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX), and octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX), their transformation products, and associated impurities is often associated with explosives manufacturing and with loading, assembling, and packing of explosives into munitions (Pugh 1982; Spaulding and Fulton 1988). Explosives may also enter the environment through training activities at firing ranges (Jenkins et al. 2000, 2001; Pennington et al. 2001b; Thiboutot et al. 1998; Thiboutot and Ampleman 2000; AMEC 2001). Quantified fate and transport parameters are required for development of remediation techniques and for risk management of explosives-contaminated sites. Not all environmental processes affect explosives transport equally; therefore, the act of identifying key processes and developing accurate numerical descriptors for these processes is critical.

Process descriptors for modeling of explosives fate and transport in soils are poorly developed because specific reaction mechanisms and their interrelations are incompletely understood (McGrath 1995). Development of process descriptor formulations has emphasized the primary explosives because of the difficulty in obtaining analytical standards and test compounds for the transformation products. An additional complication for fate and transport modeling is that all processes may not be operative in all environmental settings (Townsend and Myers 1996). For example, during subsurface transport of explosives, photolysis and volatilization are absent or minimal; however, in surface waters these processes are relevant.

Compilations of process descriptors for fate and transport of explosives have been provided in several publications (Rosenblatt et al. 1989; McGrath 1995; Brannon and Myers 1997; Talmage et al. 1999; Brannon et al. 1999). Process descriptors are also available on the Internet through the Hazardous Substance Data Base (HSDB) on the Toxicology Data Network (http://toxnet.nlm.nih.gov/). Estimation procedures are available from Boethling and Mackay (2000). Provided herein is an updated tabulation of fate and transport process descriptors for the major explosives and energetics (TNT, RDX, HMX, tetryl, picric acid, nitroglycerine, and pentaerythritol tetranitrate (PETN)), some of their principal transformation products (2ADNT, 4ADNT, 2,4DANT, 2,6DANT, 1,3,5TNB,

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1,3DNB, NB, and 3,5DNA) and some manufacturing impurities (2,4DNT, 2,6DNT) (Table 1). Pennington et al. (2001b) previously provided an overview of process descriptor data gaps and identified compounds for which additional information is needed. Work is in progress to fill these data gaps. Compounds for which no information is available, such as the nitroso transformation products of RDX, are not included in this document.

Objective

The objective of this report is to compile fate and transport process descriptors for eight energetic compounds, as well as for pertinent environmental transformation products and for impurities introduced during manufacture. The following process descriptors are included: solubility and dissolution, adsorption coefficients, transformation rates, biodegradation half-lives, photolytic half-lives, and Henry's law constants.

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2 Solubility and Dissolution

Solid phase energetic compounds can enter the environment through several mechanisms: (a) explosives/energetics manufacture, (b) munitions load, assembly, and pack, (c) munitions maintenance/demilitarization, and (d) training activities. During manufacture of explosives and during loading of explosives into ammunition shells and casings, wastewater saturated with explosives was often discharged into disposal lagoons or runoff ditches. As these waters cooled and evaporated, solid product remained on the soil surface. This product provided a reservoir for leaching of explosives through the soil profile into ground water with each rainfall event. On firing ranges the remains of munitions that have not functioned fully, e.g., failed to detonate or low order detonations, may contain significant quantities of unexploded product. Free product is available as a point source for contamination of soil and ground water. The first step in environmental transport of explosives is dissolution of these reservoirs.

Dissolution rates of solid-phase explosives describe the speed at which the explosives enter the water-soluble phase under optimal conditions of contact between the phases (Table 2). The maximum aqueous concentration that the explosive can attain at a specific temperature if the water and solid phases remain in contact long enough is the solubility (Table 3). These parameters impose limits on the mass of explosives that potentially moves in the environment as the result of rainfall events. In addition, these parameters can be used to estimate the total mass surface loading, which is a critical component of the source term needed for modeling explosives transport.

The dissolution rate for explosives and explosives formulations, such as that found inside munitions, has rarely been measured. Jenkins and Miyares have determined the dissolution rate of TNT, RDX, and HMX in a completely mixed aqueous system using estimated surface area for the explosives.[1] Results indicated the following order of dissolution rates: TNT > HMX > RDX (Table 2). Laboratory studies to determine the dissolution rates for the primary high explosives TNT, RDX, and HMX as well as formulations commonly used in munitions (Octol, Composition B, and LX14) are currently in progress (Pennington et al. 2001b).

Literature values for the aqueous solubility of explosives do not always agree (Table 3). Some of the variability may result from the level of purity and

[1] Personal Communication, T. F. Jenkins and P. H. Miyares, 3 December 1997, Cold Regions Research and Engineering Laboratory, U.S. Army Engineer Research and Development Center, Hanover, NH.

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crystalline form of the test compounds. Solubility is not always a good descriptor of the potential for transport in soils. Transport may be greatly affected by attenuation processes resulting from transformation and subsequent interaction with soil components, e.g., although TNT has a faster dissolution rate and a higher solubility than RDX, ground-water RDX plumes typically exceed the aerial extent of TNT plumes in the same aquifer. Therefore, use of a model system capable of accommodating a suite of processes is desirable for predicting transport.

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3 Adsorption

TNT

Effects of transformation on adsorption of TNT

TNT can be reversibly sorbed by soils (Haderlein, Weissmahr, and Schwarzenbach 1996; Pennington and Patrick 1990). However, reactions that remove TNT from solution and bind TNT transformation products to soil in an unextractable manner can be mistaken for adsorption (Pennington et al. 1995a; Brannon, Price and Hayes 1997; Price, Brannon, and Hayes 1997). Several investigators have reported batch-determined equilibrium sorption coefficients whose isotherms were typical of existing models (Leggett 1985; Pennington and Patrick 1990; Ainsworth et al. 1993; Xue, Iskandar, and Selim 1995; Comfort et al. 1995; Haderlein, Weissmahr, and Schwarzenbach 1996). However, recent experiments have shown that TNT in batch tests for some soils may not reach nonzero steady-state concentrations in either soil or dissolved phases due to transformations (Price, Brannon, and Hayes 1995; Myers et al. 1998). Some investigators have tried to eliminate the effects of transformation by using (a) short equilibration times (Myers et al. 1998), (b) poisoning of microbes (Ainsworth et al. 1993; Brannon, Price, and Hayes 1997), and (c) short equilibration times coupled with poisoning of microbes (Pennington and Patrick 1990).

Controlling and/or monitoring transformation in batch tests is also complicated by the need to define/control redox conditions and microbial activity in tests. Analysis of solution phase in batch tests may reflect TNT disappearance from solution by both sorption and transformation. Direct measurements of soil phase TNT concentrations have shown that steady-state is not reached in some soils because TNT continues to transform, especially under anaerobic conditions (Myers et al. 1998; Price, Brannon, and Hayes 1995). Therefore, isotherms based only on solution phase analyses may be misleading. Steady-state conditions for TNT are more likely to be attained in low organic carbon soils, such as those typical of aquifers, than in typical surface soils (Pennington et al. 2001a).

Effects of test variables on adsorption coefficients

In an uncontrolled batch experiment, redox conditions are highly variable and depend on the headspace gas, initial concentration of oxygen in the water and soil, microbial activity, organic matter, iron, manganese, sulfur, and numerous other redox-sensitive substances. TNT transformation is more rapid when

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nitrogen is the headspace gas and de-aired water is used than when redox potential is not controlled (Myers et al. 1998). When Eh is not controlled, test conditions may not exemplify conditions in the natural environment of interest and may lead to inaccurate adsorption coefficients.

TNT adsorption onto clay minerals

In some subsurface soils where redox conditions and soil properties do not promote transformation, sorption may be more important than transformation. Haderlein, Weissmahr, and Schwarzenbach (1996) reported equilibration times of 30 to 60 min and fully reversible surface adsorption of TNT and its transformation products on clay minerals. High adsorption constants were measured with homoionic K^+ or NH_4^+ clays (up to 21,500 L/kg) compared to much lower sorption (up to 1.7 L/kg) when Ca^{+2}, Na^+, Mg^{+2}, or Al^{+3} was the exchangeable cation. These results suggest that the sorption behavior in freshwater and saline waters may be very different. In freshwater environments dominated by Ca^{+2}, sorption of TNT and its transformation products to soils, sediments, and suspended sediments may be lower than that observed in a saline environment dominated by K^+ and Na^+. Therefore, the type of soil or sediment and the ionic strength and composition of the ground water or surface water are important determinants of adsorption.

Haderlein, Weissmahr, and Schwarzenbach (1996) showed that the mobility of TNT degradation products are likely to be significantly lower than TNT in subsurface environments where specific adsorption to clay minerals dominates the sorption process. Distribution coefficients for a K^+-saturated montmorillonite decreased in the order TNT > 2ADNT > 4ADNT > 2,6DANT > 2,4DANT. On the other hand, testing with a heavy clay soil showed much lower distribution coefficients and more uniform distribution (within a factor of two) for TNT and its transformation products (Myers and Townsend 1997). Therefore, depending upon the characteristics of the sorbent, TNT transformation products may either be more mobile than TNT or show similar mobility.

Competitive adsorption

Competitive adsorption between TNT, its transformation products, and other explosives has been postulated to affect sorption and transport (Loehr 1989; Ainsworth et al. 1993). Competition between adsorbed explosives was negligible only in very dilute systems. After the linear range for adsorption was exceeded on clays, explosives with a higher distribution coefficient displaced compounds with a lower distribution coefficient (Haderlein, Weissmahr, and Schwarzenbach 1996). For example, 2ADNT displaced 2,4DANT from clay sorption sites into the solution phase.

Effects of free product in soils

Because of past waste disposal practices, surface soils can present large repositories of undissolved explosives, or free product, specifically where

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explosives were manufactured, loaded, and packaged into shells. Free product is also present after low-order detonations of munitions on firing ranges. Solid explosives are relatively stable due to their slow dissolution rate (Pennington et al. 1995b; Thiboutot et al. 1998). When free product was present in batch partitioning tests, the aqueous solubility of the respective explosives controlled solution phase concentrations masking sorption behavior (Pennington et al. 1995b).

TNT adsorption coefficients

Soil adsorption coefficients for TNT vary over a range of 0 to 11 L/kg (Table 4) (Brannon et al. 1999; Pennington and Patrick 1990). Adsorption coefficients onto homoionic clays ranged up to 413 L/kg and followed a Freundlich rather than a linear isotherm model (Price et al. 2000).

Adsorption coefficients for TNT transformation products

Adsorption coefficients for the TNT transformation products, 2ADNT, 4ADNT, 2,4DANT, 2,6DANT, 1,3,5TNB, and 1,3DNB, have been measured in aquifer soils, a few surface soils, and pure clays (Pennington et al. 1995b, 1999, 2001b; Brannon et al. (in review); Brannon unpublished data; Haderlein, Weissmahr, and Schwarzenbach 1996). Values for all of the transformation products are within the same range for each medium, i.e., extremely low K_d values are observed in aquifer soils, less than 1.0 L/kg; extremely high K_d values are observed in the pure clays; and K_d values in the range of 2 to 6 L/kg are observed in surface soils (Tables 5-10).

RDX

Adsorption coefficients for RDX in soils ranged from 0 to 8.4 L/kg (Table 11). Sorption can be described by linear isotherms (Leggett 1985; Ainsworth et al. 1993; Selim and Iskandar 1994; Haderlein, Weissmahr, and Schwarzenbach 1996; Myers et al. 1998). The low adsorption coefficient suggests that adsorption will not be a significant attenuation process in the transport of RDX in typical aquifer environments. In general, RDX is sorbed less than TNT by soils (Haderlein, Weissmahr, and Schwarzenbach 1996; Townsend and Myers 1996). In comparative studies, significantly less RDX than TNT was associated with soil organic matter (Price, Brannon, and Yost 1998). Desorption was also consistent with field observations on the relative mobility of TNT and RDX, i.e., RDX was more mobile than TNT (Brannon, Price, and Hayes 1997). Although the soils were sterilized by gamma irradiation, abiotic transformation of TNT may have influenced these results.

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HMX

Substantially less data are available on the sorption of HMX than on TNT and RDX (Table 12). In general, HMX adsorption coefficients were <1 L/kg in aquifer soils, and within the range of 1 to 18 L/kg in surface soils. In column studies HMX sorption was approximately described using a linear equilibrium model (Myers et al. 1998). HMX is less sorbed and more mobile than is TNT (Townsend and Myers 1996; Price, Brannon, and Yost 1998).

Dinitrotoluenes

Little data are available on sorption of the dinitrotoluenes (Tables 13 and 14). Values for adsorption to aquifer soils were consistent with K_d values for other energetics, i.e., typically <1 L/kg (Pennington et al. 1999). Values for adsorption to pure clays were higher for 2,4DNT than for 2,6DNT (Haderlein, Weissmahr, and Schwarzenbach 1996). The Sharkey clay surface soil K_d of 12.5 L/kg (Pennington et al. 2001a) was consistent with surface soil values for TNT and TNT transformation products.

Tri- and Di-Nitrobenzenes

Adsorption coefficients for 1,3,5TNB and 1,3DNB in aquifer soils were extremely low (Tables 9 and 10, respectively). In the limited surface soil data, values for 1,3,5TNB were higher (up to 4.4 L/kg). Significant adsorption of 1,3DNB onto homoionic clay was reported (Haderlein, Weissmahr, and Schwarzenbach 1996). Additional data with surface soils are needed to adequately address mobility of these compounds.

Other Energetics

Adsorption coefficients for the remaining energetics, nitrobenzene, 3,5-dinitroaniline, tetryl, picric acid, nitroglycerine, and PETN, were not found. Available organic carbon normalized partition coefficients (K_{oc}) values for nitrobenzene, 3,5-dinitroaniline, tetryl, picric acid, nitroglycerine and PETN, as well as for other energetics, are presented in Table 15.

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4 Transformation

TNT

Transformation is the modification of a chemical substance in the environment by either biological or abiotic mechanisms. Transformation rates generally include modifications resulting from both abiotic and biotic mechanisms. Transformation rate coefficients have been determined under both aerobic and anaerobic conditions and are typically on the order of seconds to minutes (Table 16). Although TNT reductive transformation has been known for some time (McCormick, Feeherry, and Levinson 1976; Kaplan and Kaplan 1982), only recently have TNT reductive transformation products been routinely measured in laboratory and field studies (Townsend, Myers, and Adrian 1995; Price, Brannon, and Hayes 1997; Comfort et al. 1995; Selim, Xue, and Iskandar 1995; Xue, Iskandar, and Selim 1995; Haderlein, Weissmahr, and Schwarzenbach 1996; Myers et al. 1998). Possible TNT transformations include reduction of one, two, or all three of the nitro-moieties to amines, and coupling of amino transformation products to form dimers (Figure 1) (Kaplan and Kaplan 1982). Formation of the two monoamino transformation products, 2ADNT and 4ADNT, are energetically favored (Riefler and Smets 2000) and are typically observed in TNT-contaminated soils and ground water. Since the diamino products are energetically more difficult to form, they are observed less frequently and typically at lower concentration than the monoamino products (Pennington et al. 2001a). The triamino product is rarely observed not only because it is more energetically difficult to form, but also because once formed, it does not persist, but is likely to be immobilized by chemical reactions with soil components (Achtnich et al. 2000) or by microbial degradation (Lewis et al. 1996). Available transformation rate coefficients for the amino transformation products are summarized in Tables 17-20.

The amino transformation products are amenable to several attenuation mechanisms in soils. These include covalent bonding to functional groups on soil organic matter such as described for similar amines (Thorn et al. 1996a, 1996b; Ononye and Graveel 1994; Parris 1980), reactions at mineral surfaces (Klausen, Haderlein, and Schwarzenbach 1997; Weber, Spidle, and Thorn 1996; Haderlein, Weissmahr, and Schwarzenbach 1996), sequestration (Achtnich et al. 2000), and reversible adsorption (Brannon, Price, and Hayes 1997; Myers et al. 1998; Pennington and Patrick 1990; Pennington et al. 1995b). Although these mechanisms for attenuation of TNT have received attention in laboratory studies in the last several years, little data have been reported on their occurrence in the field

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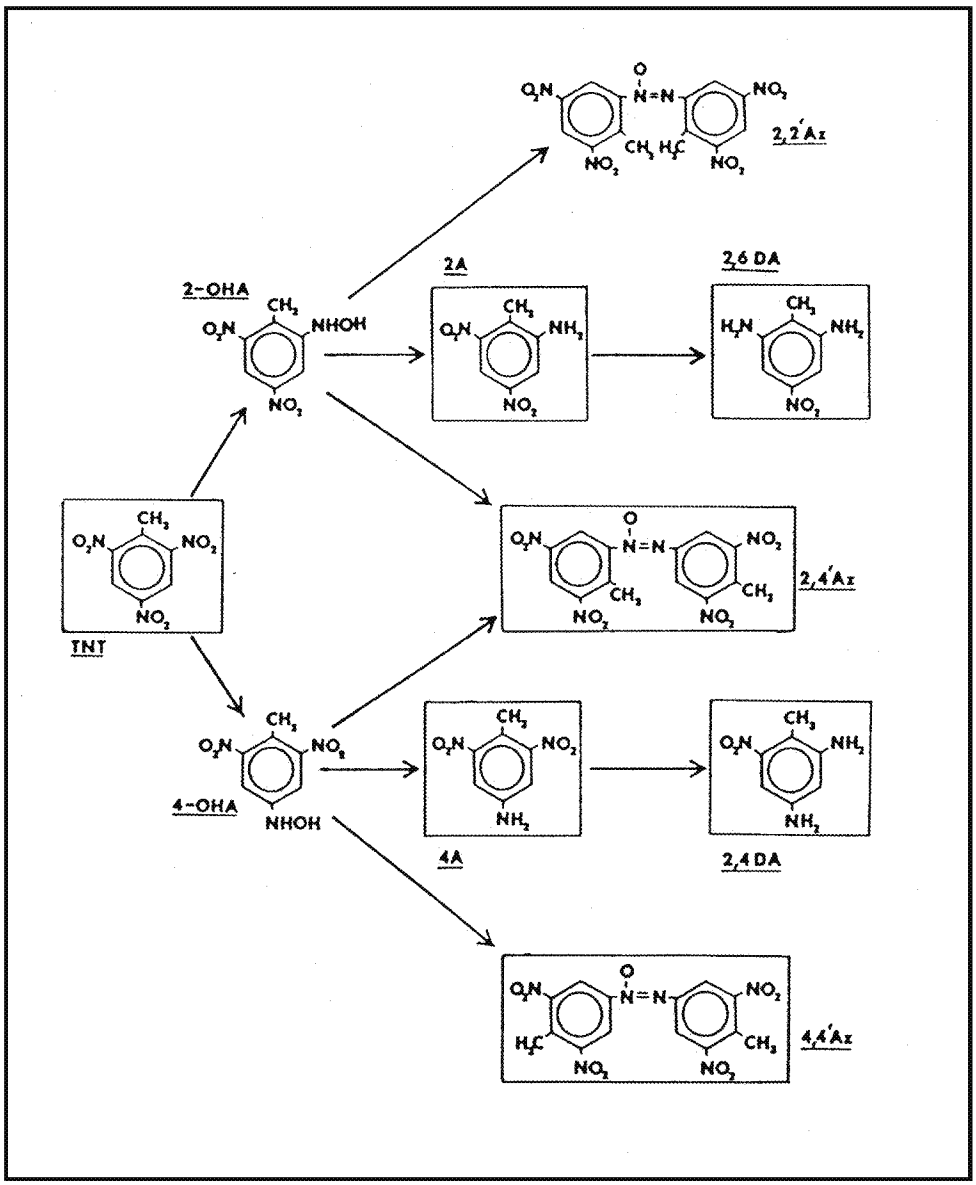

Figure 1. Biotransformation of TNT in compost (Kaplan and Kaplan 1982)

beyond detection of the amino transformation products in soil and ground water and declines in TNT concentrations over time (Pennington et al. 2001a).

Laboratory studies have demonstrated the effects of several environmental factors on transformation of TNT. Such factors include redox status, pH, organic carbon levels, cation exchange capacity, and presence/absence of expandable clays and reducing agents, e.g., divalent iron and manganese. TNT transformation is significantly enhanced under anaerobic conditions, but occurs at a slower rate under aerobic conditions (Price, Brannon, and Hayes 1995, 1997).

TNT disappeared from the solution phase of slurry tests under highly reduced conditions (Eh = -150 mV) following 1 day of incubation (Price, Brannon, and Hayes 1997). The monoamino and diamino transformation products disappeared

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rapidly in all tests at all concentrations and pH values. Under aerobic conditions (Eh = +500 mV), TNT completely disappeared from solution after 4 days compared to less than 1 day under highly reduced conditions. Only the monoamino transformation products appeared with maximum concentrations at day 4, but with detectable concentrations through day 14. These results demonstrated that TNT transformation is more rapid under highly reducing conditions (Eh = -150 mV) than under oxidizing conditions (Eh = +500 mV), but that neither TNT nor its transformation products persist under either condition.

TNT transformations in soils can occur both biologically and abiotically (Pasti-Grigsby et al. 1996; Pennington and Patrick 1990; Ainsworth et al. 1993). The rate of TNT transformation by Fe^{+2} in the presence of montmorillonite or kaolinite increased as pH increased (Brannon, Price, and Hayes 1998). Products were primarily monoamino and azoxy compounds; however, mass balances using radiolabeled TNT indicated the presence of unextractable products. Suppression of the abiotic Fe^{+2} pathway by addition of ethylene-diaminetetraacetic acid (EDTA) slowed reduction, but the suppression lasted for no more than 24 hr.

RDX

Only limited RDX transformation rate data were found (Table 21). Transformation of RDX through mono-, di-, and tri-nitroso products has been postulated (Funk et al. 1993; Crawford 1995) and observed under anaerobic conditions in soil (Price et al. 2001). Similar transformation products are produced following treatment of RDX-contaminated soil with chemical oxidants (Hawthorne et al. 2000). Such reductions lead to destabilization, ring cleavage, and mineralization of RDX under anaerobic conditions (Figure 2; McCormick, Feeherry, and Levinson 1976; McCormick, Cornell, and Kaplan 1981; Kaplan 1996). Degradation intermediates are susceptible to aerobic as well as anaerobic mineralization; however, mineralization is nearly an order of magnitude greater under anaerobic conditions (Price et al. 2001). The nitroso intermediates of RDX have rarely been observed in the field at the few sites where analyses have been conducted for them.

HMX

Little is known regarding the transformation of HMX. However, formation of mono- and di-nitroso intermediates during biotransformation has been identified (McCormick et al. 1985). In laboratory studies HMX is stable under a broad range of redox and pH conditions (Price, Brannon, and Yost 1998). First-order transformation rate constants for HMX have been measured in soil column and shake-test experiments (Townsend and Myers 1996; Price, Brannon, and Yost 1998). Rate constants ranged from 0 to 0.062 hr^{-1} (Table 22). Transformation products of HMX have rarely been detected in the environment. However, analyses for transformation products have been limited.

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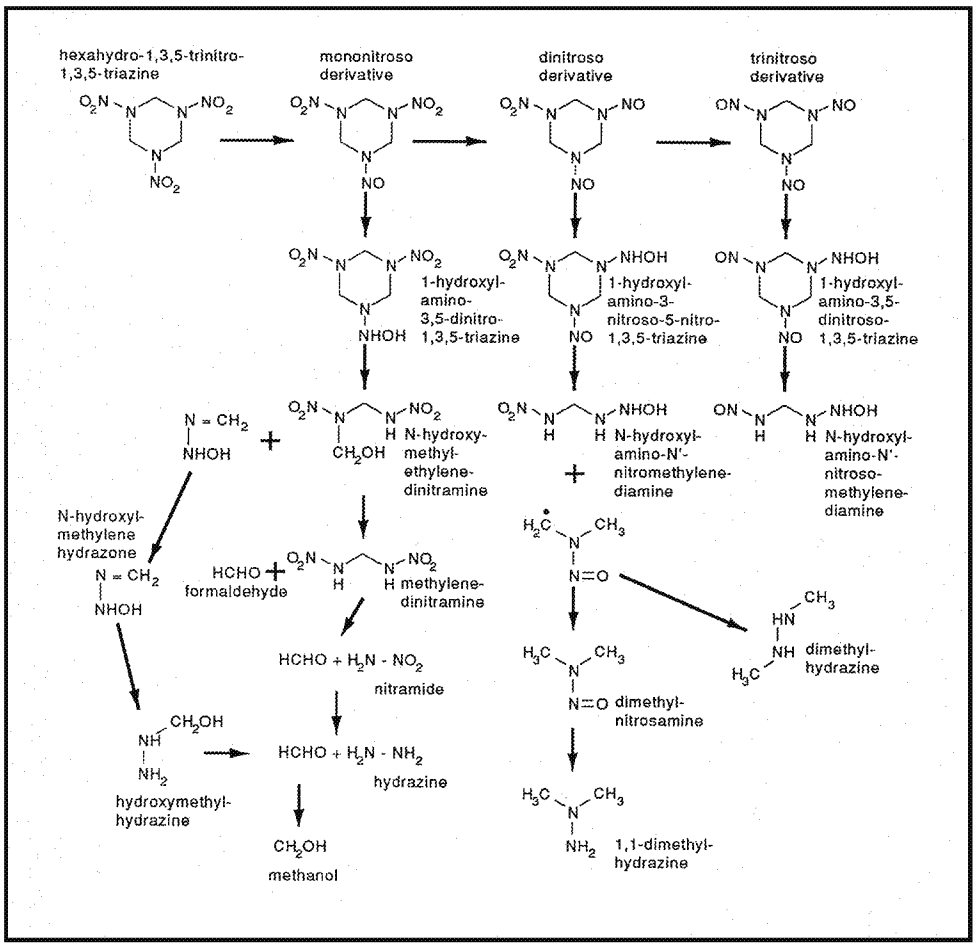

Figure 2. Anaerobic biomineralization pathway for RDX (McCormick, Feeherry, and Levinson 1976; Kaplan 1996)

Tri- and Di-Nitrobenzenes

Transformation rates for 1,3,5TNB (Tabel 23) and 1,3DNB (Table 24) are lower than rates for TNT and RDX and similar to those for HMX. However, the data for both compounds are very limited.

Dinitrotoluenes

Transformation rates for the DNTs are lower than rates for TNT, RDX, and HMX; however, data are very limited (Tables 25 and 26). Covalent bonding reactions between these aminated products and soil organic carbon functional groups are postulated. Current research by the Environmental Laboratory of the U.S. Army Engineer Research and Development Center (ERDC) and the U.S. Geological Survey, Denver, is exploring these reactions using nuclear magnetic resonance techniques.

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Other Energetics

Picric acid can undergo reduction of the nitro groups in a manner similar to TNT, especially under anaerobic conditions (Kaplan 1996; McCormick, Feeherry, and Levinson 1976). However, the limited data concerning transformation rate coefficients suggest that transformation may not occur in aquifers (Table 27).

Nitroglycerin is anaerobically biodegradable via successive denitration (Christodoulatos, Bhaumik and Brodman 1997). Intermediates included glycerol dinitrate and glycerol mononitrate. No transformation rate coefficients were found.

PETN can be transformed by sequential denitration through tri-, di-, and mono-nitrated pentaerythritol to un-nitrated pentaerythritol, which is subject to subsequent mineralization (Kaplan 1996). Binks et al. (1996) report denitration of PETN when used as a sole nitrogen source by a soil microbial isolate. Intermediate products included pentaerythritol dinitrate, 3-hydroxy-2,2'-*bis*-[(nitrooxy)methyl]propanoal, and 2,2-*bis*-[(nitrooxy)methyl]-propanedial. French, Nicklin, and Bruce (1998) report release of nitrite from TNT using the enzyme isolated from a PETN-degrading microorganism. No transformation rate coefficients were found. Four transformation products of tetryl were isolated from soils in a plant uptake study (Harvey et al. 1991). One was identified as *N*-methyl-2,4,6-trinitroaniline; one was tentatively identified as dinitrophenylmethylnitramine; two others were undefined reduction products of the first two. Transformation was a rapid and extensive process (Fellows, Harvey, and Cataldo 1993). However, no transformation rate coefficients were determined.

Immobilization of TNT

Evidence for immobilization of TNT in soils with consequent reduction in bioavailability was dramatically illustrated in a plant uptake study using TNT-amended soils (Folsom et al. 1988). Results revealed the significant reduction in bioavailability of TNT for plant uptake from clay as compared to silt. Other evidence for TNT immobilization was identified in composting experiments using [^{14}C]TNT-amended soils (Kaplan and Kaplan 1982; Caton et al. 1994; Pennington et al. 1995a). In these studies, significant quantities of unextractable radioactivity and no radiolabeled volatiles or CO_2 were observed. These results confirmed that mineralization of TNT was not occurring during composting, but that immobilization accounted for the observed dramatic reductions in TNT. Further study of the composting process demonstrated that no TNT and very few identifiable products of TNT could be released from the finished compost even with stringent base/acid hydrolysis schemes (Thorne and Leggett 1997; Pennington et al. 1997, 1998). Similar results were observed when compost was subjected to ultraviolet light and repeated aqueous leaching (Caton et al. 1994). Microbial degradation studies have shown that the immobilized products of TNT in compost are resistant to mineralization (Pennington et al. 1997, 1998). Results of nuclear magnetic resonance techniques using stable isotopes of nitrogen and carbon confirmed covalent bonding of TNT transformation products to functional

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groups on humic acid (Thorn 1997). Studies to define the factors governing the characteristics of observed products are ongoing at the ERDC in the Installation Restoration Research Program work unit entitled "Immobilization of 2,4- and 2,6-Dinitrotoluenes in Soils."

The recent focus on immobilization has supported development of remediation technologies. For example, covalent binding of reduced metabolites to soil organic matter during bioremediation has been investigated (Achtnich et al. 1999, 2000; Bruns-Nagel et al. 2000; Daun et al. 1998; Lenke et al. 1998). In these studies, the time course for disappearance of TNT and appearance and disappearance of transformation products was typically on the order of hours to days.

Immobilization of Other Energetics

Immobilization of RDX and other energetic contaminants is limited. Results of high-performance liquid chromatographic analysis of compost containing both TNT and RDX indicated much less disappearance of RDX (approximately 30 percent) than of TNT (more than 90 percent) after 20 days (Pennington et al. 1995a). Since RDX is more readily degraded under anaerobic conditions than TNT and no radiolabeled RDX was present in the tests for monitoring of $^{14}CO_2$, disappearance of RDX may have been due to mineralization rather than immobilization. In the same experiment, no significant change in HMX concentration was observed, which suggests that HMX immobilization is not significant. While relatively undocumented for the aminated products of explosives, other aromatic amines have been reported to undergo covalent binding and subsequent irreversible polymerization and rearrangement in the environment (Bollag and Myers 1992; Bollag, Myers, and Minard 1992; Hsu and Bartha 1974; Thorn et al. 1996a, 1996b).

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5 Biodegradation

TNT

Several TNT mineralization pathways have been reviewed by Crawford (1995). Anaerobic mineralization in the laboratory through triaminotoluene (TAT) to trihydroxytoluenes, polyphenols, -cresol, and acetate has been reported (Funk et al. 1993; Crawford 1995). Evidence of TNT mineralization in soils or ground water is scarce. Results of studies in which aquifer soils were challenged with ^{14}C-labeled TNT and RDX revealed that the native microflora from two sites possessed limited potential for attacking and degrading these compounds (Pennington et al. 2001a). Furthermore, the limited degradation proceeded at a very slow rate. Spanggord et al. (1980b) reported a biodegradation half-life of 19 to 25 days in water down gradient from several Army ammunitions plants, while the Agency for Toxic Substances and Disease Registry (ATSDR 1995) reported a half-life of 1 to 6 months for TNT in surface water (Table 28).

TNT Transformation Products

A recent mini-review, or comment, asserted that only biotransformation, not mineralization, of TNT has been observed in soil treatment systems (Hawari et al. 2000a). Degradation of the amino reductive products of TNT has been observed in the laboratory, but only limited degradation rate data are available (Table 28). TNT metabolism by microorganisms slated for use in bioremediation technologies has been studied extensively (Hughes et al. 1998; Crawford 1995; Daun et al. 1998; Lenke et al. 1998; Lewis et al. 1997; Hofstetter et al. 1999; Bruns-Nagel et al. 1998; Haidour and Ramos 1996).

RDX

RDX is more readily degraded than TNT, especially under anaerobic conditions (McCormick, Cornell, and Kaplan 1985; Funk et al. 1993; Regan and Crawford 1994; Coleman, Nelson, and Duxbury 1998). Final products may include methanol and hydrazines, and under methanogenic conditions, methane (McCormick, Feeherry, and Levinson 1976; Kaplan 1996; Hawari et al. 2000b). Although no half-life data were found, limited aerobic biodegradation has been

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observed in soils (Cataldo, Harvey, and Fellows 1993); complete anaerobic biodegradation has been observed under laboratory conditions (Spanggord et al. 1980a, 1980b, 1983a, 1983b). Sheremata and Hawari (2000b) report N_2O as a significant mineralization product that should be monitored at contaminated sites where biodegradation by the white rot fungus is suspected to occur.

HMX

Relatively little is known concerning the degradation of HMX, but results of the few observations suggest that HMX is recalcitrant to mineralization, yielding mono- and di-nitroso intermediates only and transforming under anaerobic conditions only (McCormick, Cornell and Kaplan 1985; Spanggord et al. 1982). Spanggord et al. (1983a) give a half-life of 17 and 1.6 hr, respectively, for aerobic and anaerobic waste stream effluent treated with yeast (Table 28). Boopathy (2001) reported degradation to methanol and chloroform under sulfate-reducing, nitrate-reducing, fermenting, methanogenic, and mixed-electron-accepting conditions using an anaerobic digester sludge enrichment culture. Rates varied from 22 ppm on day 0 to <0.05 ppm on day 11.

Dinitrotoluenes

An extensive literature base is available concerning biodegradation of dinitrotoluenes, including, but not limited to: Haidour and Ramos 1996; Nishino et al. 1999; Ortega-Calvo, Fesch, and Harms 1999; Lendenmann, Spain, and Smets 1998; Hughes, Wang, and Zhang 1999; Zhang et al. 2000; and Haidour and Ramos 1996). An excellent summary of degradation mechanisms of nitro-aromatic compounds is provided by Nishino, Spain, and He (2000). The two DNTs are described as susceptible to elimination of a nitro group ultimately yielding nitrite and catechols under aerobic conditions. A pathway is given by Nishino, Paoli, and Spain (2000). Under anaerobic conditions, cometabolic reduction of nitro groups to nitroso-, aminonitro-, diamino-, and azoxy-compounds have been observed (Liu, Thompson, and Anderson 1984; McCormick, Cornell, and Kaplan 1978; McCormick, Feeherry, and Levinson 1976; Nishino, Spain, and He 2000). As for TNT, reductive products typically represent a metabolic "dead end" precluding ring cleavage (Nishino, Spain, and He 2000). In bioreactor systems degradation rates of 86 mg 2,4DNT L^{-1} hr^{-1} have been achieved (Reardon and Spain 1993; Nishino, Spain, and He 2000). However, design of reactors to degrade mixtures of 2,4- and 2,6DNT are more challenging and a subject of current research (Nishino, Spain, and He 2000). No other degradation rate data were found.

Tetryl

Tetryl can be converted to aniline by sulfate-reducing bacteria (Boopathy 2000), but a rate was not determined.

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Tri- and Di-Nitrobenzenes

Boopathy et al. (1998) report degradation to trinitrobenzene as well as several other explosives by sulfate-reducing bacteria yielding ammonia. Davis, Boopathy, and Manning (1997) report metabolism of TNB to nitrobenzene by a *Pseudomonas* isolate. Boopathy (1994) reported transformation of TNB to amino compounds. Reduction of one or more nitro groups results in aniline for which an extensive literature addresses degradation.

Picric Acid

Picric acid is biotransformed under anaerobic conditions to picramic acid (McCormick, Feeherry, and Levinson 1976). Complete mineralization has been described by Lenke, Achtnich, and Knackmuss (2000), Lenke and Knackmuss (1992), Sariaslani and Rajan (1994), and Rajan et al. (1996). However, no data describing degradation rates in natural systems were found.

Nitroglycerine and PETN

The nitrate esters of interest as explosives include nitroglycerin, PETN, and nitrocellulose. A recent review of degradation of nitrate esters was given by Williams and Bruce (2000). Nitroglycerin, or glycerol trinitrate, can be degraded by sequential removal of nitro groups (Wendt, Cornell, and Kaplan 1978). However, the degradation did not progress further. Mineralization in both aerobic and anaerobic sludge reactors has been reported, but was slower and required substantial enrichment under aerobic conditions (Angermaier, Hein, and Simon 1981; Angermaier and Simon 1983). No environmental rate data were discovered. PETN is biodegraded by sequential denitration to pentaerythritol (Kaplan 1996; Binks et al. 1996). Degradation rates were not found.

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6 Photolysis and Volatilization

Photolysis

TNT

Photodecomposition of TNT was probably recognized from the earliest days of manufacture because of the conspicuous color change, to a red or pink, of manufacturing waste waters exposed to sunlight. The most extensive studies of TNT photochemistry were conducted by Burlinson and his co-workers (Burlinson 1980; Burlinson et al. 1973, 1979; Kaplan, Burlinson, and Sitzmann 1975) and by Spanggord and his co-workers (Spanggord et al. 1980a, 1980b; Liu, Spanggord, and Bailey 1976). Photodecomposition of TNT is much more rapid in natural sunlight than in darkness (Spanggord et al. 1980b). Concentrations of TNT in Mississippi River water neared zero after 6 to 8 days exposure to sunlight, whereas 30 days in darkness were required to dissipate 90 percent. Photodecomposition was inversely proportional to pH over the range 1.1 to 11.1 pH units. At pH 11.1, TNT decomposed even in darkness, possibly as a result of base hydrolysis. Photolysis was more rapid in river water than in distilled water (Burlinson 1980). This may have been due to the higher pH of the river water, but Spanggord et al. (1980b) submit that the effects of pH are insignificant relative to the effects of natural substances in the water. Their results indicated that light absorption by substances in natural water sensitizes TNT resulting in photolytic transformations. Similar results are reported by Mabey et al. (1983). Photolysis is greater in nonpolar than in polar solvents (Suryanarayanan and Capellos 1970, 1972, 1974). For example, the decay rate constant in benzene was more than 20,000 times greater than in methanol.

Few studies have reported photolysis products of TNT from natural waters, but Burlinson et al. (1979) identified an extensive list of products from laboratory irradiation (Table 29). Burlinson et al. (1979) reported that 45 to 50 percent of the photodecomposition products of TNT were recovered in solution (Table 29) with the remainder present as insoluble residues suggestive of oligomers of azo and azoxy compounds, which were not identified. Burlinson et al. (1979) proposed that TNT photolysis occurs through 2,4,6-trinitrobenzaldehyde, some undefined nucleophilic complex, and ultimately produces 1,3,5-trinitrobenzene.

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Photolysis affects the fate of explosives primarily in the aquatic environment, but could affect explosives exposed to sunlight on the soil surface. Available rate constants for photolysis are summarized in Table 30. Photoelectrochemical remedial techniques in reactors are not addressed in this report but are described by Schmelling, Gray, and Kamat (1996).

Other energetics

Data describing photolytic half-lives of other energetics are limited (Table 30). No half-life determinations were found for 2ADNT, 4ADNT, 2,4DANT, 2,6DANT, 3,5DNA, and PETN, while only a suggestion of the potential for photolysis was found for picric acid, nitroglycerine, 1,3DNB, and 2,6DNT. The use of ultraviolet light as a decomposition tool for the remediation of some explosives-containing wastes has been explored, typically in combination with oxidizing agents (Larson, Miller, and Crowley 1996, Lipczynska-Kochany 1992, Wang and Kutal 1995). Half-lives of energetics in ultraviolet treatment systems are not reported here.

Volatilization

The Henry's Law constant is a measure of the ratio of the concentration in the gaseous state to the concentration in aqueous solution and is key to estimating losses due to volatilization during fate and transport evaluations. Available Henry's Law constants for volatilization are summarized in Table 31.

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7 Conclusions and Recommendations

Conclusions

Process descriptors that may be of value in development of transport models and risk assessments include solubility and dissolution kinetics, transformation and adsorption rates in soils, and biodegradation rates in soils and ground water. Under some conditions, photolysis will also be significant. Process descriptors for TNT, RDX, HMX, tetryl, picric acid, nitroglycerine, PETN, and some of the transformation products of these explosives were tabulated from literature values when available. Except for transformation products of TNT and the dinitrotoluenes, aqueous solubilities for explosives are available at various temperatures. However, dissolution kinetics have rarely been measured. Determinations of dissolution kinetics for the primary high explosives and formulations of high explosives are in progress at the ERDC.

Transformation rates of the explosives TNT, RDX, HMX, picric acid, 2,4- and 2,6-dinitrotoluene, and certain transformation products of TNT, have been measured in a limited number of soils. The monoamino transformation products of TNT and some of the benzene derivatives have been observed frequently in soil and ground water at contaminated sites, but most other transformation products have been observed primarily in the laboratory. However, analytical standards for some of these compounds have not been available. Therefore, analyses for them in the environment have been limited. Recent availability of standards for transformation products of RDX has resulted in low-level detections at some sites. Transformation rates tend to be related to properties of the soils and the redox status of the system.

Adsorption coefficients for TNT have been measured in a number of soils varying widely in physical characteristics. The database for RDX, HMX, transformation products of TNT, and the dinitrotoluenes is more limited, while no data were found for nitrobenzene, tetryl, picric acid, nitroglycerine, and PETN. The extent to which explosives are adsorbed is limited, especially relative to environmental contaminants such as polychlorinated biphenyls and certain metals. Typically, adsorption is greater for TNT than for the other explosives. Separation of adsorption from transformation in typical batch tests is difficult. Therefore, some TNT adsorption rates may reflect transformation followed by

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re-equilibration of transformation products as well as adsorption of the parent compound.

Explosives have been the subject of biotransformation/biodegradation studies since the early 1980s. An extensive literature exists for degradation pathways, but less data are available on degradation rates. Degradation pathways under oxidizing and reducing conditions differ, as do degradation rates. Intermediates of some pathways have not been confirmed. Explosives span a broad range of degradation rates from very recalcitrant/slow, such as HMX, to relatively unstable/fast, such as nitroglycerine.

Most of the work concerning photolysis of explosives focused on TNT and was conducted in the 1970s. Data are also available for RDX and HMX. However, no data are available for many of the other compounds. Measured or estimated values of Henry's Law constants are available for most explosives, except for some TNT transformation products.

Recommendations

The driver for future research in this area will expand from cleanup mandates for explosives manufacturing and munitions development to sustaining military readiness by appropriately managing training and testing ranges in an environmentally responsible manner. Additional research is needed to delineate fate and transport parameters for explosives compounds for which data are limited. Adsorption and transformation rate coefficients are adequate for TNT, RDX, HMX, and the mono- and di-amino transformation products of TNT. Additional research is needed for most other explosives compounds. In addition, fate and transport parameters will also be needed for compounds associated with smokes, propellants, illuminants, organics used in fuses, fillers or stabilizers, and heavy metals on firing ranges. Assessing the potential for explosives contamination and the potential for exposure of environmental and human receptors resulting from various military activities cannot be carried out without accurate fate and transport process descriptors.

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Table 1
Explosives, Transformation Products, and Manufacturing Impurities

Compound	CAS Number[1]	Abbreviation
2,4,6-trinitrotoluene	118-96-7	TNT
Hexahydro-1,3,5-trinitro-1,3,5-triazine	121-82-4	RDX
Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine	2691-41-0	HMX
2-amino-4,6-dinitrotoluene	35572-78-2	2ADNT
4-amino-2,6-dinitrotoluene	19406-51-0	4ADNT
2,4-diamino-6-nitrotoluene	6629-29-4	2,4DANT
2,6-diamino-4-nitrotoluene	59229-75-3	2,6DANT
2,4-dinitrotoluene	121-14-2	2,4DNT
2,6-dinitrotoluene	606-20-2	2,6DNT
1,3,5-trinitrobenzene	99-35-4	1,3,5TNB
1,3-dinitrobenenze	99-65-0	1,3DNB
Nitrobenzene	98-95-3	NB
3,5-dinitroanaline	618-87-1	3,5DNA
N,2,4,6-tetranitro-N-methylaniline	479-45-8	Tetryl
2,4,6-trinitrophenol	88-89-1	Picric acid
1,2,3-propanetriol trinitrate	55-63-0	Nitroglycerine
Pentaerythritol tetranitrate	78-11-5	PETN

[1] CAS = Chemical Abstracts Service.

Table 2
Dissolution Rate of TNT, HMX, and RDX in a Completely Mixed Aqueous System Derived from Aqueous Concentration Changes Over Time[1]

Compound	Rate, $\mu g\ cm^{-2}\ hr^{-1}$	r^2
TNT	4,164	0.986
HMX	702	0.964
RDX	361	0.993

Note: Surface areas are estimated.
[1] T. F. Jenkins and P. H. Miyares, Cold Regions Research and Engineering Laboratory, U.S. Army Engineer Research and Development Center, Hanover, NH, 3 December 1997, unpublished data.

Table 3
Solubility of Energetic Compounds

Compound	Solubility, mg/L	Reference
TNT	51.3 (6 °C) (pH 6.9) 64.0 (12 °C) (pH 6.9) 88.5 (20 °C) (pH 7.3) 100.5 (25 °C) (pH 6.8) 204.5 (42 °C) (pH 6.8)	Ro et al. (1996) Other literature values are not presented because of generally close agreement with these data.
RDX	28.9 (10 °C) 42.3 (20 °C) 38.4 (20 °C) 59.9 (25 °C) 59.9 (26.5 °C) 75.7 (30 °C)	Sikka et al. (1980) Sikka et al. (1980) Spanggord et al. (1983b) Banerjee, Yalkowsky, and Valvani (1980) Sikka et al. (1980) Sikka et al. (1980)
HMX	1.21 (10 °C) 2.6 (20 °C) 5 (22-25 °C) 5.7 (30 °C) 6.6 (20 °C)	Spanggord et al. (1982b) Spanggord et al. (1982b) Glover and Hoffsommer (1973) Spanggord et al. (1982b) McLellan, Hartley, and Brower (1988)
2ADNT	2,800 (20 °C) estimated	Layton et al. (1987)
4ADNT	No data	
2,4DANT	No data	
2,6DANT	No data	
2,4DNT	270 (22 °C) 280 (25 °C)	Montgomery and Welkom (1989) Kaye (1980)
2,6DNT	208 (25 °C)	Rosenblatt et al. (1989)
1,3,5TNB	385 (25 °C) ~350 (25 °C) 340 (20 °C)	Rosenblatt et al. (1989) *The Merck Index* (1996) Spanggord et al. (1980a)
1,3DNB	469 (15 °C) 533 (25 °C) 500 (20 °C)	Verschueren (1983) Rosenblatt et al. (1989) *The Merck Index* (1996)
NB	1,797 (25 °C)	Yalkowsky and Dannenfelser (1992)
3,5DNA	Slightly soluble in cold water	Federoff et al. (1960)
Tetryl	80 (25 °C) 75 (20 °C)	Urbanski (1964) Small and Rosenblatt (1974)
Picric acid	12,400 (25 °C)	Rosenblatt et al. (1989)
Nitroglycerine	1,950 (25 °C)	U.S. Army Materiel Command (1971)
PETN	2.1 (25 °C) 43 (25 °C)	Rosenblatt et al. (1989) Rinkenback (1965)

Table 4
TNT Adsorption Coefficients (K_d) with Associated Soil Property Data

Soil	Soil Origin	K_d L/kg	CEC mmol/g	TOC %	Clay %	Reference
LAAP ML	Aquifer	0.04	3.5	0.015	5	Pennington et al. (1999)
LAAP SP-SM	Aquifer	0.09	3.6	0.015	5	
LAAP CL	Aquifer	0.27	8.1	0.162	15	
LAAP SM	Aquifer	0.17	5.5	0.02	7.5	
Norborne C	Surface	1.24	9.14	0.23	13	Ainsworth et al. (1993)
Cloudland C	Surface	0.81	5.6	0.05	30	
Westmoreland B1	Surface	0.58	6.9	0.98	13.6	
Ocala C4	Surface	4.3	33.5	0.08	33	
Burbank AP	Surface	1.04	5.5	0.5	4	
Sand	Surface	0.47	1.73	0.36	2.5	Brannon et al. (1992)
Silt	Surface	2.23	73	0.96	6.3	
Kolin soil	Surface	2.66	16.3	0.18	10.6	Xue, Iskandar, and Selim (1995)
Norwood soil	Surface	3.64	4.1	0.32	3	
Cornhuskers	Surface	4.1	35.3	0.83	20	Pennington and Patrick (1990)
Crane	Surface	3.7	31.2	2.8	20.6	
Holston A	Surface	4.4	28.8	2.7	18.1	
Holston B	Surface	3.0	35.2	1.2	43.8	
Iowa	Surface	5.2	44.7	1.4	20	
Joliet	Surface	6.8	102	3.6	23.8	
Kansas	Surface	5.7	130.4	2.6	26.3	
Lonestar	Surface	2.5	15.5	0.56	10	
Longhorn	Surface	3.7	20.9	0.56	15	
Louisiana	Surface	2.5	16.3	0.37	10.6	
Newport	Surface	2.3	13.4	3.5	5.6	
Radford	Surface	3.2	21.5	1.1	25	
Savanna	Surface	2.5	13.2	1.3	5	
Volunteer	Surface	4.05	46.4	1.7	5	
Clay	Surface	11	124.9	2.4	54.4	
Silt	Surface	2.8	17.2	0.57	17.5	
Sharkey clay	Surface	10 1.85	38.9	2.4	48.7	Townsend, Myers, and Adrian (1995) Myers et al. (1998)
WES-silt	Surface	4.5 1.77	12.4	0.57	7.5	
Ottawa sand	Surface	1.50	NM	NM	0	
Crane sifter	Surface	6.16	15	1.3	23	Pennington et al. (1995b)

(Continued)

Note: CEC = cation exchange capacity; TOC = total organic carbon; LAAP = Louisiana Army Ammunition Plant; WES = Waterways Experiment Station; NM = not measured; NA = not applicable.

Table 4 (Concluded)						
Soil	**Soil Origin**	**K_d L/kg**	**CEC mmol/g**	**TOC %**	**Clay %**	**Reference**
Agricultural topsoil	Surface	6.38	14.6	4.9	4	Sheremata and Hawari (2000a)
Agricultural topsoils	Surface	6.38-11.96	14.6	8.4	4	Sheremata et al. (2001)
Various		0-10	NA	NA	NA	Townsend and Myers (1996)
LAAP A	Surface	1.09	2.5	0.31	6	Price et al. (2000)
LAAP C	Surface	1.06	6.6	0.08	12	
LAAP D	Surface	1.67	15.5	0.2	32	
Montmorillonite	Pure clay	413	27.7	NM	NM	
Sand (Borden)	Pure sand	0.4	NM	0.02	2	Cattaneo et al. (2000)
Sand (4% clay)	Surface	1.3	NM	NM	4	
Loam	Surface	1.6	NM	NM	NM	
Kaolinite clay	Pure clay	1	NM	NM	NM	
Montmorillonite	Pure clay	156	NM	NM	NM	

Table 5 2ADNT Adsorption Coefficients (K_d) with Associated Soil Property Data						
Soil	**Source**	**K_d L/kg**	**CEC mmol/g**	**TOC %**	**Clay %**	**Reference**
LAAP A	Aquifer	NSA[1]	2.5	0.31	6	Brannon et al. (in review)
LAAP B	Aquifer	0.31	3.1	0.23	6	
LAAP C	Aquifer	0.06	6.6	0.08	12	
LAAP D	Aquifer	0.32	15.5	0.2	32	
Sharkey clay	Surface	5.54	38.9	2.4	48.7	Brannon, unpublished data
Hastings	Surface	6.22	26	1.37	28	Pennington et al. (1995b)
Sand (Borden)	Surface	1[2]	NM	0.02	2	Cattaneo et al. (2000)
Sand (4% clay)	Surface	18[2]	NM	NM	NM	
K^+-kaolinite	Pure clay	300	0.3	NM	NM	Haderlein, Weissmahr, and Schwarzenbach (1996)
K^+-illite	Pure clay	1700	1.6	NM	NM	
K^+-montmorillonite	Pure clay	2900	12	NM	NM	

[1] No significant adsorption.
[2] Freundlich-type isotherms (n = 0.94 to 0.97).

Table 6
4ADNT Adsorption Coefficients (K_d) with Associated Soil Property Data

Soil	Source	K_d L/kg	CEC mmol/g	TOC %	Clay %	Reference
LAAP A	Aquifer	0.48	2.5	0.31	6	Brannon et al. (in review)
LAAP B	Aquifer	0.22	3.1	0.23	6	
LAAP C	Aquifer	0.29	6.6	0.08	12	
LAAP D	Aquifer	0.56	15.5	0.2	32	
Sharkey clay	Surface	4.03	38.9	2.4	48.7	Brannon (unpublished data)
Hastings	Surface	6.06	26	1.37	28	Pennington et al. (1995b)
Sand (Borden)	Surface	1[1]	NM	0.02	2	Cattaneo et al. (2000)
Sand (4% clay)	Surface	16[1]	NM	NM	NM	
K^+-kaolinite	Pure clay	11	0.3	NM	NM	Haderlein, Weissmahr, and Schwarzenbach (1996)
K^+-illite	Pure clay	70	1.6	NM	NM	
K^+-montmorillonite	Pure clay	125	12	NM	NM	

[1] Freundlich-type isotherms (n = 0.94 to 0.97).

Table 7
2,4DANT Adsorption Coefficients (K_d) with Associated Soil Property Data

Soil	Source	K_d L/kg	CEC mmol/g	TOC %	Clay %	Reference
LAAP A	Aquifer	NSA[1]	2.5	0.31	6	Brannon et al. (in review)
LAAP B	Aquifer	0.08	3.1	0.23	6	
LAAP C	Aquifer	0.04	6.6	0.08	12	
LAAP D	Squifer	0.18	15.5	0.2	32	
Sharkey clay	Surface	2.05	38.9	2.4	48.7	Brannon (unpublished data)
K^+-montmorillonite	Pure clay	3.5	12	NM	NM	Haderlein, Weissmahr, and Schwarzenbach (1996)

[1] No significant adsorption.

Table 8
2,6DANT Adsorption Coefficients (K_d) and Associated Soil Property Data

Soil	Source	K_d L/kg	CEC mmol/g	TOC %	Clay %	Reference
LAAP A	Aquifer	0.06	2.5	0.31	6	Brannon et al. (in review)
LAAP B	Aquifer	0.09	3.1	0.23	6	
LAAP C	Aquifer	0.17	6.6	0.08	12	
LAAP D	Aquifer	0.35	15.5	0.2	32	
Sharkey clay	Surface	5.47	38.9	2.4	48.7	Brannon (unpublished data)
K^+-kaolinite	Pure clay	1.1	0.3	NM	NM	Haderlein, Weissmahr, and Schwarzenbach (1996)
K^+-illite	Pure clay	7	1.6	NM	NM	
K^+-montmorillonite	Pure clay	10.5	12	NM	NM	

Table 9
1,3,5TNB Adsorption Coefficients (K_d) and Associated Soil Property Data

Soil	Source	K_d L/kg	CEC mmol/g	TOC %	Clay %	Reference
LAAP ML	Aquifer	0.16	3.5	0.015	5	Pennington et al. (1999)
LAAP SP-SM	Aquifer	0.21	3.6	0.015	5	
LAAP CL	Aquifer	0.49	8.1	0.162	15	
LAAP SM	Aquifer	0.27	5.5	0.02	7.5	
Hastings	Surface	2.90	26	1.37	28	Pennington et al. (1995b)
Weldon Springs	Surface	4.38	18	3.11	19	
K^+-montmorillonite	Pure clay	>60000	12	NM	NM	Haderlein, Weissmahr, and Schwarzenbach (1996)

Table 10
1,3DNB Adsorption Coefficients (K_d) and Associated Soil Property Data

Soil	Source	K_d L/kg	CEC mmol/g	TOC %	Clay %	Reference
LAAP ML	Aquifer	0	3.5	0.015	5	Pennington et al. (1999)
LAAP SP-SM	Aquifer	0	3.6	0.015	5	
LAAP CL	Aquifer	0.32	8.1	0.162	15	
LAAP SM	Aquifer	0	5.5	0.02	7.5	
Sharkey clay	Surface	17.7	38.9	2.4	48.7	Pennington et al. (2001)
K^+-montmorillonite	Pure clay	4500	12	NM[4]	NM	Haderlein, Weissmahr, and Schwarzenbach (1996)

Table 11
RDX Adsorption Coefficients (K_d) with Associated Soil Property Data[1]

Soil	K_d L/kg	CEC mmol/g	TOC %	Clay %	Reference
LAAP ML	0.21	3.5	0.015	5	Pennington et al. (1999)
LAAP SP-SM	0.33	3.6	0.015	5	
LAAP CL	0.33	8.1	0.162	15	
LAAP SM	0.33	5.5	0.02	7.5	
Elk-B1	0.27	6.92	0.45	16.5	Ainsworth et al. (1993)
Cloudland C	0.12	5.6	0.05	30	
Cecil AP	0.43	4.88	0.59	62	
Cecil BT	0.31	2.92	0.32	53	
Burbank Ap	0.16	5.5	0.5	4	
Kenoma BC	0.93	31.4	0.5	44	
Kenoma Bt1	1.21	26	1.43	44	
Ocala C4	2.37	33.5	0.08	33	
Watson 2Bxg	1.45	10.3	0.4	47	
Westmoreland A1	1.65	6.91	2.03	14.4	
	2.39	73.4	6.04	38.2	Tucker et al. (1985)
	0.81	39.3	0.54	30.3	
	0.5	27.7	0.32	10.3	
	2.42	41.8	6.32	0.8	
	7.3	14.5	3.1	3.8	
	0.07	0.7	0.18	0.2	
	0.74	8.7	1.22	10.7	
	0.57	2.9	0.1	4.8	
	0.06	22	0.23	30.1	
	0.7	19	0.4	37.8	
	0.57	44.7	0.98	22.2	
	0.87	41.5	0.66	20.3	
Sand	0.29	1.73	0.36	2.5	Brannon et al. (1992)
Silt	1.20	73	0.96	6.3	
Rathbun (extracted)	8.4	114	0.92	16.5	
Kolin soil	1.59	16.3	0.18	10.6	Xue, Iskandar, and Selim (1995)
Norwood soil	1.57	4.1	0.32	3	
Yokena clay	3.5	38.9	2.4	48.7	Brannon, unpublished data
West end	2.2	45.7	0.18	7.5	
Yuma	1.07	5.4	0.04	5.0	
D Street	0.82	1.8	0.17	0.0	
Yokena clay	0.95	38.9	2.4	34	Myers et al. (1998)
WES-silt	0.77	12.4	0.57	7.5	
Ottawa sand	0	NM	NM	0	
Sharpsburg A horizon	0.97	18.3	1.7	36	Singh et al. (1998)
Sharpsburg C horizon	0.95	19	0.4	32	
Agricultural topsoil	6.38[2]	14.6	4.9	4	Sheremata et al. (2001)
Various	0.2-7.8	NA	NA	NA	Townsend and Myers (1996)
LAAP D	0.29	15.5	0.2	32	Price et al. (2000)

[1] All soils are surface soils.
[2] Freundlich coefficient, n = 1.1.

Table 12
HMX Adsorption Coefficients (K_d) with Associated Soil Property Data

Soil	Source	K_d L/kg	CEC mmol/g	TOC %	Clay %	Reference
LAAP ML	Aquifer	0.086	3.5	0.015	5	Pennington et al. (1999)
LAAP SP-SM	Aquifer	0.20	3.6	0.015	5	
LAAP CL	Aquifer	0.37	8.1	0.162	15	
LAAP SM	Aquifer	0.20	5.5	0.02	7.5	
LAAP D	Aquifer	2.39	15.5	0.2	32	Price et al. (2000)
Browns Lake	Surface	7.42	15.3	0.38	10.0	Brannon et al. (1999)
Sharkey clay	Surface	12.1	38.9	2.40	48.8	
St. Mary Parish, LA	Surface	17.7	14.2	0.19	20	
Picatinny B	Surface	4.25	9.8	0.634	5	
Socorro S	Surface	3.25	34.0	0.08	35	
Socorro P	Surface	1.17	27.3	0.12	27.5	
Grange Hall silt	Surface	0.12	16.7	0.29	10	
Yuma 1B	Surface	5.02	8.6	0.03	5	
China Lake	Surface	1.65	3.5	0.02	5	
Sharkey clay	Surface	1.6	38.9	2.4	48.7	Myers et al. (1998)[1]
WES-silt	Surface	1.17	12.4	0.57	7.5	
Ottawa sand	Surface	0	NM	NM	0	
Holston River	Sediment	8.7	NM	1.3	NM	McGrath (1995)
Montmorillonite	Pure clay	4.99	13.2	0.19	30	Brannon et al. (1999)

[1] Column study.

Table 13
2,4DNT Adsorption Coefficients (K_d) and Associated Soil Property Data

Soil	Source	K_d L/kg	CEC mmol/g	TOC %	Clay %	Reference
LAAP ML	Aquifer	0.09	3.5	0.015	5	Pennington et al. (1999)
LAAP SP-SM	Aquifer	0.28	3.6	0.015	5	
LAAP CL	Aquifer	0.67	8.1	0.162	15	
LAAP SM	Aquifer	NSA[1]	5.5	0.02	7.5	
LAAP D	Aquifer	1.67	15.5	0.2	32	Pennington et al. (2001a)
Sharkey clay	Surface	12.5	38.9	2.4	48.7	
K^+-kaolinite	Pure clay	690	0.3	NM	NM	Haderlein, Weissmahr, and Schwarzenbach (1996)
K^+-illite	Pure clay	3650	1.6	NM	NM	
K^+-montmorillonite	Pure clay	7400	12	NM	NM	

[1] No significant adsorption.

Table 14
2,6DNT Adsorption Coefficients (K_d) and Associated Soil Property Data

Soil	Source	K_d L/kg	CEC mmol/g	TOC %	Clay %	Reference
LAAP C	Aquifer	0.96	6.6	0.08	12	Pennington et al. (2001a)
LAAP D	Aquifer	1.83	15.5	0.2	32	
Sharkey clay	Surface	5.96	38.9	2.4	48.7	
K^+-kaolinite	Pure clay	10	0.3	NM	NM	Haderlein, Weissmahr, and Schwarzenbach (1996)
K^+-illite	Pure clay	52	1.6	NM	NM	
K^+-montmorillonite	Pure clay	125	12	NM	NM	

Table 15
K_{oc} of Energetic Compounds

Compound	Log K_{oc}	Reference
TNT	3.2	Spanggord et al. (1980b)
RDX	0.88 – 2.4	Sikka et al. (1980) Burrows et al. (1989) Spanggord et al. (1980b) Tucker et al. (1985)
HMX	2.8	Spanggord et al. (1982b)
2ADNT	No data available	
4ADNT	No data available	
2,4DANT	No data available	
2,6DANT	No data available	
2,4DNT	1.79[1] – 2.4	Montgomery and Welkom (1989) Rosenblatt et al. (1989)
2,6DNT	1.79[1] – 1.89[1]	Montgomery and Welkom (1989) Rosenblatt et al. (1989)
1,3,5TNB	1.8 – 2.7	Spanggord et al. (1980a) ASTDR (1995) Lyman, Reehl, and Rosenblatt (1982)
1,3DNB	1.8 – 2.3	Spanggord et al. (1980a) U.S. Army (1987)
NB	1.48 – 2.57	Seip et al. (1986) Loekke (1984) Wilson et al (1981) Walton et al (1992) Kopinke et al (1995)
3,5DNA	2.4 – 2.7	Von Oepen, Kordel, and Klein (1991)
Tetryl	1.69 – 2.6 (calculated) 3.1 – 3.5	Burrows et al. (1989) Syracuse Research Corporation (1995) Hale, Stanford, and Taft (1979)
Picric acid	2.00[1]	Rosenblatt et al. (1989)
Nitroglycerine	1.66 - 2.77[1]	Rosenblatt et al. (1989)
PETN	3.39[1]	Rosenblatt et al. (1989)

[1] Estimated value.

Table 16
TNT Soil Transformation Rate Coefficients (*K*), Oxidation Status During Test, and Soil Properties

Soil	Oxidation Status	*K* hr^{-1}	CEC mmol/g	TOC %	Clay %	Reference
LAAP B	Aerobic	0	3.6	0.015	5	Brannon et al. (in review)
LAAP B	Anaerobic	0.0003	3.6	0.015	5	
LAAP D	Aerobic	0.0006	15.5	0.2	32	
LAAP D	Anaerobic	0.0016	15.5	0.2	32	
LAAP CL	Anaerobic	0.0014	8.1	0.162	15	Pennington et al. (1999)
LAAP ML	Anaerobic	0.0006	3.5	0.015	5	
LAAP SM	Anaerobic	0.0007	5.5	0.02	7.5	
LAAP SP-SM	Anaerobic	0.0006	3.6	0.015	5	
Sharkey clay	Aerobic	0.0163	38.9	2.4	48.7	Brannon and Myers (1997)
Sharkey clay	Anaerobic	0.062	38.9	2.4	48.7	
Clay + Fe^{++}	Anaerobic	0.011 (pH 6) 0.072 (pH 7) 4.36 (pH 8)	NA	NA	NA	Brannon, Price, and Hayes (1998)
Various	Various	0.0017 – 0.0087	NA	NA	NA	Ainsworth et al. (1993)
WES-silt	Aerobic	0.025	12.4	0.57	7.5	Townsend, Myers, and Adrian (1995)
Yokena clay	Aerobic	0.013	38.9	2.4	34	
Ottawa sand	Aerobic	0.008	NM	NM	0	
WES-silt	Aerobic	0.144	12.4	0.57	7.5	Myers et al. (1998)
Yokena clay	Aerobic	0.162	38.9	2.4	34	
Ottawa sand	Aerobic	0.003	NM	NM	0	
LAAP D	Aerobic	0.008	15.5	0.20	32	Price et al. (2000)

Table 17
2ADNT Soil Transformation Rate Coefficients (*K*), Oxidation Status During Test, and Soil Properties

Soil	Oxidation Status	*K* hr^{-1}	CEC mmol/g	TOC %	Clay %	Reference
LAAP B	Aerobic	0	3.6	0.015	5	Brannon et al. (in review)
LAAP B	Anaerobic	0	3.6	0.015	5	
LAAP D	Aerobic	0.0006	15.5	0.2	32	
LAAP D	Anaerobic	0.0016	15.5	0.2	32	
LAAP ML	Anaerobic	0.0004	3.5	0.015	5	Pennington et al. (1999)
LAAP SP-SM	Anaerobic	0.0003	3.6	0.015	5	
LAAP CL	Anaerobic	0.0011	8.1	0.162	15	
LAAP SM	Anaerobic	0.0005	5.5	0.02	7.5	
Sharkey clay	Aerobic	0.0067	38.9	2.4	48.7	Brannon and Myers (1997)
Sharkey clay	Anaerobic	0.048	38.9	2.4	48.7	

Table 18
4ADNT Soil Transformation Rate Coefficients (*K*), Oxidation Status During Test, and Soil Properties

Soil	Oxidation Status	*K* hr^{-1}	CEC mmol/g	TOC %	Clay %	Reference
LAAP B	Aerobic	0.0026	3.6	0.015	5	Brannon et al. (in review)
LAAP B	Anaerobic	0	3.6	0.015	5	
LAAP D	Aerobic	0.032	15.5	0.2	32	
LAAP D	Anaerobic	0	15.5	0.2	32	
Sharkey clay	Aerobic	0.011	38.9	2.4	48.7	Brannon and Myers (1997)
Sharkey clay	Anaerobic	0.047	38.9	2.4	48.7	

Table 19
2,4DANT Soil Transformation Rate Coefficients (*K*), Oxidation Status During Test, and Soil Properties

Soil	Oxidation Status	*K* hr^{-1}	CEC mmol/g	TOC %	Clay %	Reference
LAAP B	Aerobic	0.0008	3.6	0.015	5	Brannon et al. (in review)
LAAP B	Anaerobic	0.0094	3.6	0.015	5	
LAAP D	Aerobic	0.0006	15.5	0.2	32	
LAAP D	Anaerobic	0.0094	15.5	0.2	32	
Sharkey clay	Aerobic	0.021	38.9	2.4	48.7	Brannon and Myers (1997)
Sharkey clay	Anaerobic	0.013	38.9	2.4	48.7	

Table 20
2,6DANT Soil Transformation Rate Coefficients (*K*), Oxidation Status During Test, and Soil Properties

Soil	Oxidation Status	*K* hr^{-1}	CEC mmol/g	TOC %	Clay %	Reference
LAAP B	Aerobic	0.0006	3.6	0.015	5	Brannon et al. (in review)
LAAP B	Anaerobic	0.0032	3.6	0.015	5	
LAAP D	Aerobic	0.004	15.5	0.2	32	
LAAP D	Anaerobic	0.0068	15.5	0.2	32	
Sharkey clay	Aerobic	0.0167	38.9	2.4	48.7	Brannon and Myers (1997)
Sharkey clay	Anaerobic	0.034	38.9	2.4	48.7	

Table 21
RDX Soil Transformation Rate Coefficients (*K*), Oxidation Status During Test, and Soil Properties

Soil	Oxidation Status	*K* hr^{-1}	CEC mmol/g	TOC %	Clay %	Reference
LAAP ML	Anaerobic	0	3.5	0.015	5	Pennington et al. (1999)
LAAP SP-SM	Anaerobic	0	3.6	0.015	5	
LAAP CL	Anaerobic	0.0003	8.1	0.162	15	
LAAP SM	Anaerobic	0.00009	5.5	0.02	7.5	
Sharkey clay	Aerobic	0.0163	38.9	2.4	48.7	
Sharkey clay	Anaerobic	0.062	38.9	2.4	48.7	
Sharkey clay	Aerobic	0 - 0.008	38.9	2.4	48.7	Price, Brannon, and Yost (1998)
Sharkey clay	Anaerobic	0.12 - 0.24	38.9	2.4	48.7	
Various	Various	0.0017 - 0.0087	NA	NA	NA	Ainsworth et al. (1993)
WES-silt	Aerobic	0.006	12.4	0.57	7.5	Myers et al. (1998)
Yokena clay	Aerobic	0.008	38.9	2.4	34	
Ottawa sand	Aerobic	0	NM	NM	0	
LAAP D	Aerobic	0.008	15.5	0.20	32	Price et al. (2000)

Table 22
HMX Soil Transformation Rate Coefficients (*K*), Oxidation Status During Test, and Soil Properties

Soil	Oxidation Status	*K* hr^{-1}	CEC mmol/g	TOC %	Clay %	Reference
LAAP ML	Anaerobic	0	3.5	0.015	5	Pennington et al. (1999)
LAAP SP-SM	Anaerobic	0	3.6	0.015	5	
LAAP CL	Anaerobic	0.00044	8.1	0.162	15	
LAAP SM	Anaerobic	0	5.5	0.02	7.5	
Sharkey clay	Aerobic	0.0163	38.9	2.4	48.7	Brannon and Myers (1997)
Sharkey clay	Anaerobic	0.062	38.9	2.4	48.7	
Sharkey clay	Aerobic	0 - 0.04	38.9	2.4	48.7	Price, Brannon, and Yost (1998)
Sharkey clay	Anaerobic	0 - 0.05	38.9	2.4	48.7	
Various	Various	0.0017 - 0.0087	NA	NA	NA	Ainsworth et al. (1993)
WES-silt	Aerobic	0.004	12.4	0.57	7.5	Myers et al. (1998)
Yokena clay	Aerobic	0.016	38.9	2.4	34	
Ottawa sand	Aerobic	0	NM	NM	0	

Table 23
1,3,5TNB Soil Transformation Rate Coefficients (*K*), Oxidation Status During Test, and Soil Properties

Soil	Oxidation Status	*K* hr^{-1}	CEC mmol/g	TOC %	Clay %	Reference
LAAP ML	Anaerobic	0.0006	3.5	0.015	5	Pennington et al. (1999)
LAAP SP-SM	Anaerobic	0.0006	3.6	0.015	5	
LAAP CL	Anaerobic	0.0027	8.1	0.162	15	
LAAP SM	Anaerobic	0.0005	5.5	0.02	7.5	
Sharkey clay	Aerobic	0.18	38.9	2.4	48.7	Pennington et al. (2001)
Ground water/soil	Not specified	Probable	NM	NM	NM	McGrath (1995)

Table 24
1,3DNB Soil Transformation Rate Coefficients (*K*), Oxidation Status During Test, and Soil Properties

Soil	Oxidation Status	*K* hr^{-1}	CEC mmol/g	TOC %	Clay %	Reference
LAAP ML	Anaerobic	0	3.5	0.015	5	Pennington et al. (1999)
LAAP SP-SM	Anaerobic	0.0019	3.6	0.015	5	
LAAP CL	Anaerobic	0.0013	8.1	0.162	15	
LAAP SM	Anaerobic	0.0019, 0.0001	5.5	0.02	7.5	
Sharkey clay	Anaerobic	0.0476	38.9	2.4	48.7	Pennington et al. (2001)
Ground water	Not specified	0.001 (estimated)	NM	NM	NM	Howard et al. (1991)
Soil	Not specified	0.001 - 0.002 (estimated)	NM	NM	NM	

Table 25
2,4DNT Soil Transformation Rate Coefficients (*K*), Oxidation Status During Test, and Soil Properties

Soil	Oxidation Status	*K* hr^{-1}	CEC mmol/g	TOC %	Clay %	Reference
LAAP ML	Anaerobic	0.017	3.5	0.015	5	Pennington et al. (1999)
LAAP SP-SM	Anaerobic	0.0017	3.6	0.015	5	
LAAP CL	Anaerobic	0.0021	8.1	0.162	15	
LAAP SM	Anaerobic	0.0021	5.5	0.02	7.5	
Sharkey clay	Anaerobic	Rapid	38.9	2.4	48.7	Pennington et al. (2001)
Ground water	Anaerobic	0.0001[1]	NM	NM	NM	Howard et al. (1991)
Ground water	Aerobic	0.0144[1]	NM	NM	NM	
Soil	Not specified	0.0002 – 0.0015[1]	NM	NM	NM	

[1] Estimated.

Table 26
2,6DNT Soil Transformation Rate Coefficients (*K*), Oxidation Status During Test, and Soil Properties

Soil	Oxidation Status	*K* hr^{-1}	CEC mmol/g	TOC %	Clay %	Reference
LAAP C	Anaerobic	0.0023	6.6	0.08	12	Pennington et al. (2001)
LAAP D	Anaerobic	0.0035	15.5	0.2	32	
Sharkey clay	Anaerobic	0.0235	38.9	2.4	48.7	
Ground water	Anaerobic	0.0001[1]	NM	NM	NM	Howard et al. (1991)
Ground water	Aerobic	0.0144[1]	NM	NM	NM	
Soil	Not specified	0.0002 – 0.0015[1]	NM	NM	NM	

[1] Estimated.

Table 27
Picric Acid Transformation Rate Coefficients (*K*), Oxidation Status During Test, and Properties of Aquifer Soils Used in the Tests

Soil	Oxidation Status	*K* hr^{-1}	CEC mmol/g	TOC %	Clay %	Reference
LAAP ML	Anaerobic	0	3.5	0.015	5	Pennington et al. (1999)
LAAP SP-SM	Anaerobic	0	3.6	0.015	5	
LAAP CL	Anaerobic	0.0037	8.1	0.162	15	
LAAP SM	Anaerobic	0	5.5	0.02	7.5	

Table 28
Biotransformation/Biodegradation Rates of Energetics in Various Media

Compound	Rates, Half Lives ($t_{1/2}$), and Comments	Reference
TNT	TNT transformed in soils and other media under both aerobic and anaerobic conditions 19-25 days	Price, Brannon, and Hayes (1997) Spanggord et al. (1980b)
RDX	Limited aerobic degradation in soils Biodegradation occurs under anaerobic conditions	Cataldo, Harvey, and Fellows (1993) Spanggord et al. (1980b) Spanggord et al. (1983b)
HMX	$t_{1/2}$ = 17 hr and 1.6 hr, respectively, in aerobic and anaerobic waste stream effluent treated with yeast Removal from 22 ppm on day 0 to <0.05 ppm on day 11 under sulfate-reducing, nitrate-reducing, fermenting, methanogenic, and mixed electron-accepting conditions with enrichment cultures from anaerobic digester sludge	Spanggord et al. (1983a) Boopathy (2001)
2ADNT	$t_{1/2}$ = 50 hr (white rot fungus) $t_{1/2}$ = 170 hr (bacterial culture)	Bumpus and Tatarko (1994) Alvarez et al. (1995)
4ADNT	No data available	
2,4DANT	No data available	
2,6DANT	No data available	
2,4DNT	Under aerobic conditions up to 80% reduction in 28 days, of which 28% is mineralized; under anaerobic conditions some methanogenic bacteria can degrade 50% - 98% in 30 days	9 references in HSDB (2001)
2,6DNT	Aerobic conditions: $t_{1/2}$ = 73 – 92 days in soils; variable results in other media. Anaerobic conditions: some methanogenic bacteria can degrade 55% - 95% in 30 days	13 references in HSDB (2001)
1,3,5TNB	24% disappearance in 19 days in river water:sediment mixture.	Mitchell, Dennis, and Burrows (1982)
1,3DNB	$t_{1/2}$ = 1 day in Tennessee River water following 10-day lag phase; $t_{1/2}$ = 9.7 days in laboratory enrichment cultures	Mitchell and Dennis (1982) Mitchell, Dennis, and Burrows (1982)
Nitrobenzene	Degradation results are conflicting with results ranging from rapid degradation to no degradation	14 references in HSDB (2001)
3,5DNA	Following 12-day lag phase, 33% - 52% concentration decrease in water containing sediments	Mitchell, Dennis, and Burrows (1982)
Tetryl	No information on microbial degradation, but microbial reduction of nitro groups to amines occurs readily	Layton et al. (1987)
Picric acid	Results suggest that picric acid is resistant to aerobic degradation, but it has been shown to undergo transformation under anaerobic conditions in pure cultures	8 references in HSDB (2001)
Nitroglycerine	0.15 – 1.88 days (anaerobic growth media) 53.6% loss in 5 days (activated sludge inoculum)	Christodoulatos, Bhaumik, and Brodman (1997) Wendt, Cornell, and Kaplan (1978)
PETN	No data available	

Table 29
Photodecomposition Products of TNT

Compound	Reference
1,3,5-trinitrobenzene	Burlinson et al. (1973); Spanggord et al. (1980a); Kaplan, Burlinson, and Sitzmann (1975); Epstein, Sommer, and Hackley (1978)
2,4,6-trinitrobenzaldehyde	Burlinson et al. (1973); Burlinson et al. (1979); Spanggord et al. (1980a); Kaplan, Burlinson, and Sitzmann (1975); Epstein, Sommer, and Hackley (1978)
4,6-dinitroanthranil	Burlinson et al. (1973); Burlinson et al. (1979); Spanggord et al. (1980a); Epstein, Sommer, and Hackley (1978)
2,4,6-trinitrobenzonitrile	Burlinson et al. (1973); Burlinson et al. (1979); Spanggord et al. (1980a); Kaplan, Burlinson, and Sitzmann (1975)
2,2',6,6'-tetranitro-4,4'-azoxytoluene	Burlinson et al. (1973)
4,4',6,6'-tetranitro-2,2'-azoxytoluene	Burlinson et al. (1973)
2',4-dimethyl-3,3',5,5'-tetranitro-ONN-azoxybenzene	Burlinson et al. (1973)
2,4'-dimethyl-3,3',5,5'-tetranitro-ONN-azoxybenzene	Burlinson et al. (1979)
2,4-dinitroisoanthranil	Burlinson et al. (1979)
2,2'-dicarboxy-3,3'5,5'-tetranitroazobenzene	Burlinson et al. (1979); Kaplan, Burlinson, and Sitzmann (1975)
2-carboxy-3,3'5,5'-tetranitro-NNO-azoxybenzene	Burlinson et al. (1979); Kaplan, Burlinson, and Sitzmann (1975)
2-amino-4,6-dinitrobenzoic acid	Burlinson et al. (1979); Spanggord et al. (1980a); Kaplan, Burlinson, and Sitzmann (1975)
4,6-dinitroisoanthranil	Kaplan, Burlinson, and Sitzmann (1975)
4,6-dinitroanthranil	Kaplan, Burlinson, and Sitzmann (1975)
Syn-2,4,6-trinitrobenzyl doxime	Kaplan, Burlinson, and Sitzmann (1975)
2,4,6-trinitrobenzyl alcohol	Kaplan, Burlinson, and Sitzmann (1975); Epstein, Sommer, and Hackley (1978)
3,5-dinitrophenol	Kaplan, Burlinson, and Sitzmann (1975); Epstein, Sommer, and Hackley (1978)
2,2'-dicarboxyl-3,3',5,5'-tetranitroazoxybenzene	Kaplan, Burlinson, and Sitzmann (1975)
2,4,6-trinitrobenzoic acid	Kaplan, Burlinson, and Sitzmann (1975)
N-(2- carboxy-3,5-dinitrophenyl)-2,4,6-trinitrobenzamide	Kaplan, Burlinson, and Sitzmann (1975)
4,6-dinitro-1,2-benzisoxazole	Epstein, Sommer, and Hackley (1978)

Table 30
Photolysis of Energetics

Compound	Findings	Reference
TNT	Half-life ($t_{1/2}$): 0.5 - 22 hr	Spanggord et al. (1980b) Mabey et al. (1983)
RDX	$t_{1/2}$ = 9 hr - 14 days, various aqueous media	Spanggord et al. (1980b) Spanggord et al. (1983b) Burrows, Chyrek, and Noss (1984) Sikka et al. (1980)
HMX	First order k = 0.15 day ($t_{1/2}$ = 5 days) $t_{1/2}$ = 1.4 - 70 days, various aqueous media	Spanggord et al. (1980b) Spanggord et al. (1982b) Spanggord et al. (1983b)
2ADNT	No data available	
4ADNT	No data available	
2,4DANT	No data available	
2,6DANT	No data available	
2,4DNT	$t_{1/2}$ = 23 - 72 hr $t_{1/2}$ = 2.7 - 43 hr, various aqueous media	Mill and Mabey (1985) Spanggord et al. (1980a)
2,6DNT	Probably important based on 2,4-DNT results	Spanggord et al. (1980a)
1,3,5TNB	Photostable Potential to photolyze	Rosenblatt et al. (1989) Mill and Mabey (1985)
1,3DNB	Not expected to be significant $t_{1/2}$ = 23 days	Spanggord et al. (1978) Simmons and Zepp (1986)
Nitrobenzene	$t_{1/2}$ = 133 days	Simmons and Zepp (1986)
3,5DNA	No data available	
Tetryl	95.4% disappearance of 12 mg/L in 20 days; hydrolysis also a significant process in water	Kayser, Burlinson, and Rosenblatt (1984)
Picric acid	Potential for direct photolysis	Kearney and Kaufman (1975)
Nitroglycerine	Probable, but no data available	Spanggord et al. (1980b)
PETN	No data available	

Table 31
Henry's Law Constants (K_H) for Explosives

Compound	K_H	Reference
TNT	1.1×10^{-8} atm m^3/mole, 25 °C (est.) 0.18 torr L/mol < 0.2 torr L/mol 4.57×10^{-7} atm m^3/mole, 20 °C	Rosenblatt et al. (1989) Spanggord et al. (1980a) Haynes and Smith (1981) Lyman, Reehl, and Rosenblatt (1982)
RDX	1.96×10^{-11} atm m^3/mole, 25 °C (est.) 2×10^{-5} torr L/mol, °C (est.)	Rosenblatt et al. (1989) Spanggord et al. (1980a)
HMX	2.6×10^{-15} atm m^3/mole, 25 °C (est.)	Rosenblatt et al. (1989)
2ADNT	3×10^{-3} torr L/mol, 20 °C (est.)	Layton et al. (1987)
4ADNT	No data	
2,4DANT	No data	
2,6DANT	No data	
2,4DNT	1.86×10^{-7} atm m^3/mole, 25 °C (est.) 1.3×10^{-7} atm m^3/mole[1]	Rosenblatt et al. (1989) Simmons and Zepp (1986)
2,6DNT	~4.86×10^{-7} atm m^3/mole, 25 °C (est.) 9.26×10^{-8} atm m^3/mole (est.)	Rosenblatt et al. (1989) Meylon and Howard (1991)
1,3,5TNB	2.21×10^{-9} atm m^3/mole, 25 °C (est.) 3.08×10^{-9} atm m^3/mole, 25 °C (est.)	Rosenblatt et al. (1989) Lyman, Reehl, and Rosenblatt (1982)
1,3DNB	8.01×10^{-7} atm m^3/mole, 25 °C (est.) 2.3×10^{-6} atm m^3/mole, 20 °C	Rosenblatt et al. (1989) Spanggord et al. (1980b)
Nitrobenzene	2.4×10^{-5} atm m^3/mole	Warner, Cohan, and Ireland (1987)
3,5DNA	No data	
Tetryl	2.69×10^{-11} atm m^3/mole, 25 °C (est.) 1.0×10^{-11} atm m^3/mole (est.)	Rosenblatt et al. (1989) Hine and Mookerjee (1975)
Picric acid	1.7×10^{-8} atm m^3/mole, 25 °C (est.)	Gorontzy et al. (1994)
Nitroglycerine	2.71×10^{-7} atm m^3/mole, 25 °C (est.)	Rosenblatt et al. (1989)
PETN	1.07×10^{-9} atm m^3/mole, 25 °C (est.) 1.2×10^{-11} atm m^3/mole, 25 °C (est.)	Rosenblatt et al. (1989) Rinkenback (1965)

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14. ABSTRACT
Waste disposal practices associated with military production of weapons, especially before and during World War II, have resulted in significant contamination of soils and ground water with high explosives such as 2,4,6-trinitrotoluene (TNT), hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX), and octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX). Development of remediation and risk management strategies for these contaminated sites as well as development of approaches for sustainable use of active training and weapons testing sites require an understanding of how the energetic compounds interact with the environment. Factors affecting fate and transport such as adsorption, microbial degradation, dissolution kinetics, solubility, and photolysis are determinants of ultimate environmental fate and exposure potential. This report summarizes the current understanding of these interactions, identifies significant data deficiencies, and provides updated process descriptors for primary explosives, transformation products, and impurities.

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