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Dissolution kinetics of sub-millimeter Composition B detonation residues: Role of particle size and particle wetting

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ABSTRACT

The dissolution of the 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) from microscale particles (<250 μm) of the explosive formulation Composition B was examined and compared to dissolution from macroscopic particles (>0.5 mm). The dissolution of explosives from detonation soot was also examined. The measured mass transfer coefficients for the microscale particles were one to two orders of magnitude greater than the macroscopic particles. When normalized to particle surface area, mass transfer coefficients of microscale and macroscale particles were similar, indicating that the bulk dissolution processes were similar throughout the examined size range. However, an inverse relationship was observed between the particle diameter and the RDX:TNT mass transfer rate coefficient ratio for dry-attritted particles, which suggests that RDX may be more readily dissolved (relative to TNT) in microscale particles compared to macroscale particles. Aqueous weathering of larger Composition B residues generated particles that possessed mass transfer coefficients that were on the order of 5- to 20-fold higher than dry-attritted particles of all sizes, even when normalized to particle surface area. These aqueous weathered particles also possessed a four-fold lower absolute zeta-potential than dry-attritted particles, which is indicative that they were less hydrophobic (and hence, more wettable) than dry-attritted particles. The increased wettability of these particles provides a plausible explanation for the observed enhanced dissolution. The wetting history and the processes by which particles are produced (e.g., dry physical attrition vs. aqueous weathering) of Composition B residues should be considered when calculating mass transfer rates for fate and transport modeling.

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1. Introduction

US Department of Defense (DoD) testing and training activities result in the release of various explosives on live fire ranges. One explosive formulation, Composition B, has been widely used, and contains a mixture of TNT, RDX, and HMX. These compounds typically persist in soil. RDX is particularly problematic due to its relatively high dissolved mobility in the subsurface, and has been detected in groundwater at several sites (Jenkins et al., 2001; Clausen et al., 2004; Yamamoto et al., 2004; Lewis et al., 2009; Martel et al., 2009).

To further assess the sources of these dissolved contaminants on live fire ranges, the production of residues from detonations of munitions has been examined with increased comprehensiveness in recent years. Microscale particles (and also soot) are known to be deposited at the detonation point, especially during high order detonation scenarios. For instance, controlled high-order detonations of mortar rounds produced residues that ranged from a low of <0.00001% up to a high of 2% of the original charge mass, while low-order detonations produced residues representing up to 40% of the original charge mass (Taylor et al., 2004, 2006). Residues ranged from cm-sized chunks to partially melted mm-sized particulates. The fate of these macroscopic (>1 mm) residues has been assessed in terms of aging and dissolution (Dontsova et al., 2009; Taylor et al., 2009a,b; Walsh et al., 2010).

In assessing the dissolution of mm-sized energetic residues, both Lever et al. (2005) and Taylor et al. (2009a,b) showed that the RDX content of the particle becomes enriched during dissolution due to the preferential dissolution of TNT. Consistent with this, Wang et al. (2011) used visualization techniques to confirm that microscale Composition B particles became enriched in RDX during the dissolution process.

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Although material on the order of 50 μm in size was detected from some detonations (Taylor et al., 2004), the properties of residues in the colloidal size range have not been extensively studied. These microscopic particles represent a very high surface area fraction, and as such, could contribute significantly to the mass flux of explosives at ranges. In addition, microscale residues could be more mobile than larger particles, resulting in spreading of the "source term" of explosives from the point of detonation both horizontally across the area and vertically into the soil profile. This research was undertaken to examine microscale particles of Composition B, with specific attention to their dissolution characteristics and explosive mass transfer kinetics.

2. Materials and methods

2.1. Chemicals

An artificial rainwater (ARW) based on precipitation chemistry in the northeast region of the United States, as measured by the National Atmospheric Deposition Program, was used (Wang et al., 2011). The ionic strength of ARW was ~0.3 mM and the pH was 5.0 ± 0.5. All chemicals were reagent grade or purer.

The largest amount of Composition B detonation residues were provided by the Naval Explosive Ordnance Disposal Technology Division (EODTECHDIV, Blossom Point, MD). Residues 1 cm in size or greater were collected by hand from the blast area after low-order detonation of 81- and 155-mm mortar rounds using a plasma disruptor (est. 50–80% yield). Hand-sorted residues in the size range of 0.5 to 1 mm from blow-in-place detonation of a 55-mm mortar round were a gift from Dr. Susan Taylor at the US Army Corp of Engineers Engineer Research and Development Center/Cold Regions Research and Engineering Laboratory. Additional residues, and soot from a high-order detonation, were generated by the Detonation Mechanics Laboratory at the Naval Air Warfare Center Weapons Division, China Lake via controlled detonation of blocks of Composition B. Briefly, the acceptor Composition B charge was suspended underwater inside a 20 L plastic bucket by copper wire. A donor charge (two 2.5 cm × 5.1 cm diameter Pentolite charges) was also suspended by copper wire at the correct standoff distance from the Composition B. The bucket was placed in an open air detonation chamber and detonated remotely. Residue and soot were collected by hand from the floor of the chamber after each detonation. Full details of Composition B detonations performed at China Lake are given in the online Supplementary Material. Undetonated Composition B was also supplied by China Lake.

Larger cm-sized pieces of EODTECHDIV Composition B were broken into sub mm-sized particles by three methods: physical attrition, milling, and aqueous weathering. Physical attrition consisted of grinding Composition B residues, followed by size-separation by sieving based on a previously published soil attrition method (McGee et al., 1999) with minor modifications. Briefly, about 5 g of mm-sized energetic residues were placed in a small glass jar along with solvent-cleaned stainless steel cylinders (10 × 16 mm or 13 × 13 mm). The jar was shaken on an orbital shaker at 260 rpm for 3 h. The resulting material was sieved using the US standard sieves #35 (500 μm), #60 (250 μm), #120 (125 μm), #325 (45 μm), and #635 (20 μm). The three smallest size fractions (20–45 μm, 45–125 μm, 125–250 μm) were collected and used for these studies. Milling was performed using a ceramic ball mill and ceramic stones. Small quantities of Composition B were added and milled at room temperature for 72 h. Both dry milling and wet milling (1:3 Composition B:water (w:w)) was performed, and undetonated Composition B was also milled for some studies. The term "wet-milled" is used here simply for convenience of distinguishing the various materials, and was in no real way similar to the process of aqueous weathering described next in terms of the Composition B: water ratio or the actual physical system.

Aqueous weathering was performed by manual size-reduction of residues through a 20 mesh steel screen (~800 μm opening), followed by mixing 1.5 g of Composition B with 1.8 L of purified water in a 2 L Bellco μ-Carrier spinner flask (Vineland, NJ, USA). Stirring speed averaged 250 rpm over the course of several weeks, generating a range of particle sizes through both dissolution and disintegration of the Composition B material. Based on the solubilities of the explosives and the proportions of the explosives in the Composition B, it was calculated that approximately 8% of the initial HMX and RDX, and 37% of the initial TNT, dissolved during the aqueous weathering process. Particles were concentrated from the mixing solution 40-fold by serial centrifugation (500 rpm, 25 °C, 20 min) prior to use in dissolution experiments.

2.2. Particle analyses

Ratios of HMX, RDX, and TNT in the parent Composition B materials and the generated particles were measured by five replicate extractions of small subsamples (<5 mg) in acetonitrile for 18 h in a cooled ultrasonic bath, followed by HPLC analysis (see below).

Microscale Composition B particles were analyzed using a Elzone II 5390 particle size analyzer (Micrometritics Instrument Corporation, Norcross, GA, USA). Both 30 μm and 380 μm orifice tubes were used to allow a large range of sizes to be measured. Analyses were performed in a ~2% NaCl solution saturated with HMX, RDX, and TNT to minimize particle dissolution during measurement (unless otherwise noted). A minimum of triplicate measurements were performed on each sample.

The zeta-potential and contact angle of a subset of the particle types was determined using procedures as described previously (Wang et al., 2011).

2.3. Effect of particle type and size on dissolution

Explosive dissolution from different types of microscale Composition B particles, as well as 0.5 to 1 mm residue particles for comparison, were performed by placing small amounts (~2 mg) of the material into the female luer inlet of a 13 mm glass microfiber syringe filter unit (0.45 μm pore size; Whatman 6818-1304, GE Healthcare Biosciences, Pittsburgh, PA, USA). The male luer outlet of another syringe filter was then inserted, trapping the particles between the two filters. A flow of ARW was directed into the top filter unit at a rate of 1 $\mathrm{mL\,h^{-1}}$ (calculated linear velocity across the particles on the filter of 2.4 $\mathrm{cm\,h^{-1}}$) using a syringe pump. Effluent from the filters passed through an 18 gauge stainless steel needle directly into a 2-mL vial (or a 20-mL vial during longer sampling intervals). Effluent volume was measured, and samples were analyzed for dissolved explosive concentrations by HPLC (see below). A minimum of triplicate dissolution experiments were performed with each particle type.

2.4. Explosives analysis

The concentrations of the explosives and their breakdown products were monitored during incubation using HPLC according to a modified EPA Method 8330 (http://www.epa.gov/epawaste/hazard/testmethods/sw846/pdfs/8330a.pdf) using a Dionex 3000 Ultimate HPLC with a Agilent Zorbax Bonus-RP column (4.6 × 75 mm, 3.5 μm particle diameter, 80 Å pore diameter), variable wavelength detector (254 nm), and a photodiode array detector collecting peak spectral data. The Zorbax Bonus-RP stationary phase is composed of densely reacted, sterically protected diisopropyl-C14 groups bonded to an ultrapure SiO_2 support and triple endcapped. The

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