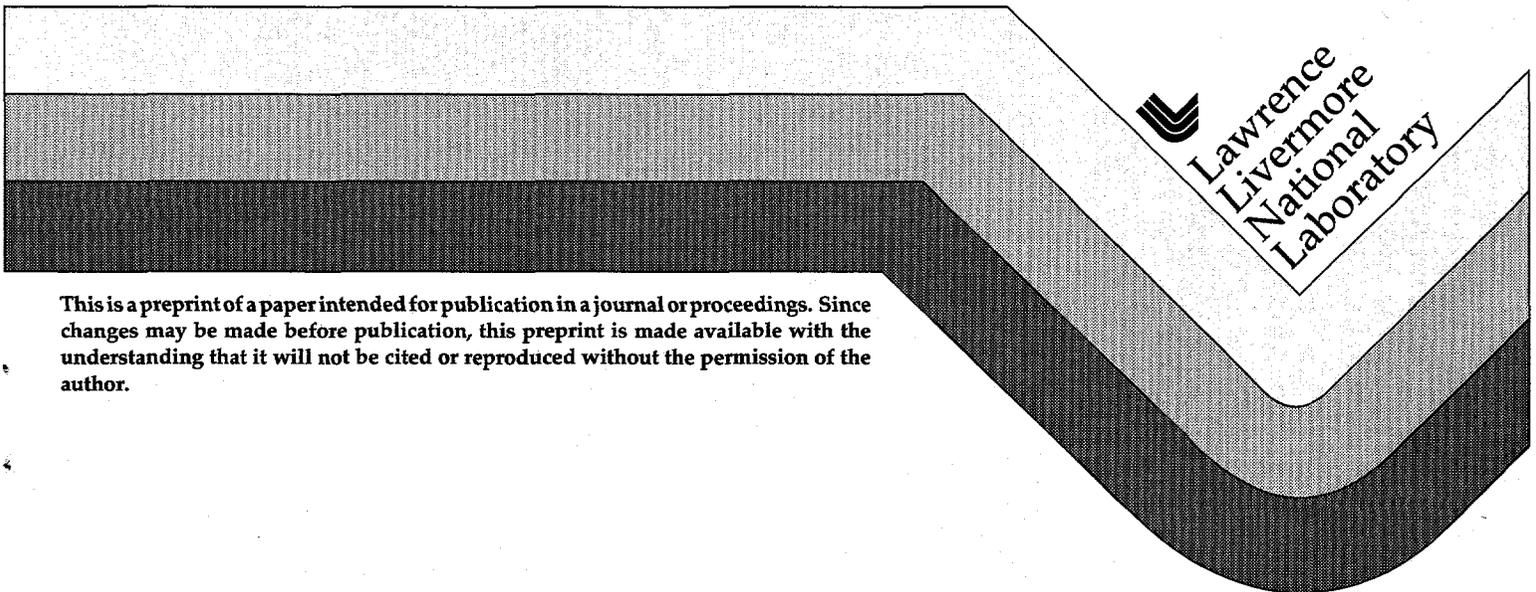


**HUMAN HEALTH RISKS  
FROM TNT, RDX, and HMX  
IN ENVIRONMENTAL MEDIA  
AND CONSIDERATION OF THE  
U.S. REGULATORY ENVIRONMENT**

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HUMAN HEALTH RISKS FROM TNT, RDX, AND HMX IN ENVIRONMENTAL MEDIA AND  
CONSIDERATION OF THE U.S. REGULATORY ENVIRONMENT

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## ABSTRACT

Although the most economical method for disposing of unwanted energetic high explosives [HEs; e.g., 2,4,6-trinitrotoluene (TNT), hexahydro-1,3,5-trinitro-triazine (RDX, also known as Cyclonite), and octahydro-1,3,5,7-tetrazocine (HMX, also known as Octogen)] involves open burning and open or underground detonation [OB/O(U)D]; federal, state, and even local government agencies in the United States (U.S.) are implementing stricter environmental regulations that eventually may prevent such activities. These stricter regulations will promote alternative technologies that are designed to be environmentally benign. However, past HE-waste disposal practices at manufacturing and fabrication facilities in the U.S. have included uncontrolled OB/O(U)D, as well as direct surface discharge of HE-contaminated waste water, resulting in contaminated environmental media (e.g., ground water, soil, and perhaps even edible vegetation) near residential areas. Using TNT, RDX, and HMX as examples, this paper describes how risk-based standards for HEs can be derived that account for potential multimedia exposures (associated with contaminated air, water, food, and soil) by individuals near a contaminated site, and used to (1) protect public health and safety, (2) prevent limited resources from being dedicated to unnecessary cleanup activities, and (3) identify the most cost-effective, practical, and environmentally benign technologies suitable for integrating with the handling of the large quantity of high explosives scheduled for demilitarization.

## INTRODUCTION

The safe disposal environmentally of high explosive (HE) compounds generated as waste during their manufacturing, testing, stockpiling, inventory reduction, assembly into or dismantlement from conventional and nuclear weapons has only recently become a priority in the United States (U.S.). For example, the established and probably most economical methods for destroying unwanted HEs are open burning and open or underground detonation [OB/O(U)D]. Depending on the locality and exact legislation, however, these activities may be limited severely or even eliminated completely in the near future by the implementation of stricter federal, state, and even local regulations designed to protect local and regional air quality. Additionally, in the U.S. Code of Federal Regulations (specifically 40 CFR, Part 261), HE-laden activated carbon that is produced as a consequence of the treatment of HE-contaminated waste water is defined to be a hazardous waste based on its reactivity.<sup>1</sup> Therefore, this hazardous solid waste either must be disposed of properly, which can be expensive, or must be rendered benign environmentally by a process that is safer and more economical than hazardous-waste disposal.

The air-quality and hazardous-waste regulations just mentioned are recent developments. Prior to enactment or consideration of these regulations, HE-waste-disposal procedures at facilities in the U.S. conducting HE manufacturing and testing and/or weapon fabrication

and/or disassembly included uncontrolled OB/O(U)D, as well as direct surface discharge of HE-contaminated waste water to unlined lagoons and ponds. The latter practice, especially, produced HE-contaminated media (e.g., ground water, soil, and perhaps even edible vegetation) near residential areas. Accordingly, it is becoming apparent that now or in the immediate future such contaminated sites will have to be evaluated for the risks or hazards the residual HE presents to human health and to what degree, if any, cleanup of the HE should be required. Although there was one effort made to provide the U.S. Army with guidance for protecting water quality from RDX contamination at its installations<sup>2</sup>, there are no federal or state regulatory limits, such as maximum contaminant levels (MCLs) or maximum contaminant level goals (MCLGs), proposed or promulgated at this time for concentrations of HEs in either soil or water that are analogous to the maximum contaminant levels (MCLs) that are an integral part of U.S. drinking water regulations [see summary of current U.S. Environmental Protection Agency (USEPA) primary and secondary standards for regulated contaminants in drinking water<sup>3</sup>]. Therefore, responsible parties accountable for the mitigation of hazardous-waste sites contaminated with HE cannot compare the concentration of a HE detected in the soil at one of these locations to a regulatory limit to rapidly ascertain whether the measured soil concentration might pose an unacceptable level of risk or hazard to public health.

To overcome the aforementioned dilemma, we have adapted a strategy that has been used to derive risk-based cleanup criterion for chemicals introduced into soil.<sup>4,5</sup> This strategy accounts for the multimedia and multipathway exposure characteristics of contaminants following their introduction into soil and is illustrated below using the energetic HE compounds 2,4,6-trinitrotoluene (TNT), hexahydro-1,3,5-trinitro-triazine (RDX or Cyclonite), and octahydro-1,3,5,7-tetrazocine (HMX or Octogen), as examples. Accordingly, the cleanup criterion determined for each of these HEs (1) protects public health and safety, (2) prevents limited resources from being dedicated to unnecessary cleanup activities, and (3) helps identify the most cost-effective, practical, and environmentally benign technologies suitable for integration with the handling of the large quantity of high explosives scheduled for demilitarization. Included in the total are over 150 metric tonnes of RDX/TNT and HMX explosives from only the expected dismantlement of nuclear weapons in the U.S. over the next ten years.<sup>6</sup>

## **MODELING THE ENVIRONMENTAL PARTITIONING OF HE INTRODUCED INTO SOIL**

To some degree, depending on the physicochemical properties of the chemical itself (including molecular weight, vapor pressure, solubility, partitioning coefficients, and intermedia transfer factors) and the characteristics of the regional landscape (including factors such as climate, geohydrology, area of contamination, and land use), a chemical introduced into the soil of that landscape will eventually distribute into multiple environmental media (e.g., air and ground water). The multimedia transport and transformation model GEOTOX<sup>7,8</sup>, which was developed at the Lawrence Livermore National Laboratory in California, U.S., was used to derive equilibrium concentrations of TNT, RDX, and HMX in soil, air, and water following their steady state input to the upper-soil layer of a 100-km<sup>2</sup> landscape representing the central-northeastern ecoregion of the U.S.<sup>9</sup> (This landscape was selected for this example because it is considered representative of many of the industrialized areas of the world.) The concentrations of RDX, HMX, and TNT predicted by the GEOTOX model for the central-northeastern ecoregion of the U.S.<sup>9</sup> and scaled to reflect unit input to the upper soil [e.g., 1 ppm

(mg/kg)] appear in Table 1. Table 2 contains the physicochemical properties of each HE compound used for predicting dose to humans following multipathway exposures.

### PATHWAY-EXPOSURE FACTORS AND MATRIX OF TERMS

Pathway-exposure factors (PEFs) designed to account for human physiology, human-behavior patterns, and environmental transport are used to connect environmental concentrations of a chemical to potential exposure pathways and lifetime accumulations. For example, the PEF for ingestion of drinking water ( $F_{ww}$ ) is obtained using Eq. 1 (see Table 3 for complete matrix of PEFs):

$$F_{ww} = I_w/B_w, \quad (1)$$

where

$I_w$  = the lifetime-equivalent fluid intake (2 L/d); and

$B_w$  = the lifetime-equivalent body weight (58 kg).

In this paper we use the PEFs developed by McKone and Daniels<sup>10</sup> to translate the predicted environmental concentrations of TNT, RDX, and HMX into quantitative estimates of amounts that could be entering the lungs, the gastrointestinal tract, and crossing the surface of the skin of exposed individuals living near the contaminated site over the course of a lifetime. For purposes of these calculations, such amounts of exposure represent applied (not metabolic) doses and are expressed in units of mg/(kg•d). A matrix containing the algebraic terms and mathematical expressions for each of the PEFs appears in Table 3. The product of a PEF term, appearing in Table 3, and the applicable concentration of a particular HE, obtained from Table 1, yields a numerical value for the dose that is associated with that HE, from that environmental media, and by that route of exposure. For each HE, the multimedia dose from a particular route of exposure is simply the sum of the doses from all environmental media (i.e., across a row in the matrix appearing in Table 3). The doses derived for both the pathway-specific multimedia exposure and the total multimedia, multipathway exposure for each HE compound are presented in Table 4. The total-exposure dose is the sum of the doses from inhalation exposure ( $E_h$ ), all ingestion exposures ( $E_g$ ), and dermal exposure ( $E_d$ ) and represents the chronic daily intake (CDI) over the course of a 70-y lifetime.

### CANCER RISK AND NONCARCINOGENIC HAZARD

The exposure-pathway-specific cancer potency (slope) factors (CPF), which are the upper-bound probabilities of an individual developing cancer (carcinogenic potency) from chronic exposure to the low dose levels of environmental concern over a 70-y lifetime, and reference doses (RfDs), which represent acceptable daily intakes associated with 70-y lifetime exposures, for each of the three HE compounds are presented in Table 5. Cancer risk is the product of the applied dose and applicable CPF. The sum of these risks constitutes the total risk to an individual. As defined by the USEPA, the ratio of the total calculated multipathway, multimedia exposure dose, expressed as the CDI, to the RfD is the hazard index.<sup>17</sup> Because only the oral RfDs are available for TNT, RDX, and HMX, we use these values in our calculations.<sup>15,16</sup>

### DETERMINING RISK AND HAZARD-BASED SOIL CONCENTRATIONS

The first step in determining possible risk- and hazard-based criteria for the cleanup of soils contaminated with the HEs of interest is to calculate the total carcinogenic risk and noncarcinogenic-hazard index associated with a 1 mg/kg

concentration of each energetic material in a soil. These values are then used to derive a range of soil concentrations for consideration as possible cleanup criteria for these compounds. The range of risk-based alternatives we derive corresponds to two levels of excess individual-lifetime cancer risk: 1 per 10,000 (i.e.,  $10^{-4}$ ) and one per 1,000,000 (i.e.,  $10^{-6}$ ). These risk levels constitute the upper boundary and goal, respectively, for potentially acceptable levels of risk cited by the USEPA<sup>19</sup> for carcinogenic substances present in environmental media. The hazard index we propose as a cleanup criterion should not exceed unity (i.e.,  $CDI/RfD \leq 1.0$ ).

For a 100-km<sup>2</sup> landscape in the central-northeastern ecoregion of the U.S., the calculated total risk associated with 1 mg/kg of an HE in soil [ $R_{TC}$  (1 mg/kg)] is derived using Eq. 2:

$$R_{TC} (1 \text{ mg/kg}) = (E_h \times CPF_h) + (E_g \times CPF_g) + (E_d \times CPF_d), \quad (2)$$

where

- $R_{TC}$  (1 mg/kg) = the *calculated* total risk associated with 1 mg/kg of HE in soil;
- $E_h$  = inhalation intake related to multimedia exposure resulting from a soil-based HE concentration of 1 mg/kg;
- $E_g$  = ingestion intake related to multimedia exposure resulting from a soil-based HE concentration of 1 mg/kg;
- $E_d$  = dermal contact intake related to multimedia exposure resulting from a soil-based HE concentration of 1 mg/kg;
- $CPF_h$  = slope factor describing cancer potency for the inhalation pathway  $[(\text{mg}/(\text{kg}\cdot\text{d}))^{-1}]$ ;
- $CPF_g$  = slope factor describing cancer potency for the ingestion pathway  $[(\text{mg}/(\text{kg}\cdot\text{d}))^{-1}]$ ; and
- $CPF_d$  = slope factor describing cancer potency for the dermal-uptake pathway  $[(\text{mg}/(\text{kg}\cdot\text{d}))^{-1}]$ .

## ALTERNATIVE SOIL-CLEANUP CONCENTRATIONS

We calculate a concentration for TNT, RDX, and HMX in soil above which cleanup is recommended,  $C_{s[\text{cleanup}]_c}$  (where  $c = r$  for risk and  $h$  for hazard), for a specific total allowable carcinogenic risk,  $R_{TA}$  (e.g.,  $10^{-6}$  or  $10^{-4}$ ), and for a noncarcinogenic-hazard index equal to 1.0. By scaling the steady-state concentration for each HE in soil,  $C_s(1 \text{ mg/kg})$ , by the ratio of  $R_{TA}$  (cleanup) to  $R_{TC}$  (1 mg/kg), we obtain the  $C_{s[\text{cleanup}]_r}$ ; by scaling  $C_s(1 \text{ mg/kg})$  by the ratio of a hazard index of 1.0 to the

quotient of the CDI and RfD, we obtain the  $C_{s[\text{cleanup}]_h}$ . Equations 3 and 4 are the mathematical expressions that define these relationships.

$$C_{s[\text{cleanup}]_r} = C_s(1 \text{ mg/kg}) \times [R_{TA}(\text{cleanup})/R_{TC}(1 \text{ mg/kg})], \text{ and} \quad (3)$$

$$C_{s[\text{cleanup}]_h} = C_s(1 \text{ mg/kg}) \times \left[ \frac{1.0}{\text{CDI}/\text{RfD}} \right]. \quad (4)$$

The concentrations of the HEs in soil that should not be exceeded are presented in Table 6 as cleanup criteria for the risk levels of  $10^{-4}$  or  $10^{-6}$  and for a hazard index of unity.

## RESULTS

The concentrations presented in Table 6 for the HEs of concern suggest that because of the possible human carcinogenicity of RDX and TNT, land contaminated with these energetic compounds at concentrations above  $0.35 \mu\text{g/kg}$  and  $2.4 \mu\text{g/kg}$ , respectively, for a  $10^{-6}$  excess cancer risk, will need to be cleaned up. These levels above which cleanup is recommended improve by two orders of magnitude, if the acceptable level for excess cancer risk is increased to  $10^{-4}$ . Nevertheless, the cancer potency of RDX is nearly an order of magnitude greater than that for TNT, and as long as TNT and RDX are considered possible human carcinogens the hazard index approach cannot be pursued because those concentrations are even above the ones associated with the excess lifetime cancer risk of  $10^{-4}$ .

However, if further toxicological studies showed these compounds not to be human carcinogens (in fact, for TNT the evidence of human carcinogenicity remains inadequate<sup>15</sup>), then the levels for cleanup would revert to the ones associated with the hazard index. Comparing the cleanup levels based on the hazard index alone (see Table 6) indicates that HMX is the least hazardous by virtue of a cleanup threshold more than one order of magnitude greater than that for RDX and almost two orders of magnitude higher than that for TNT. From the standpoint of deterministic adverse health effects, TNT appears to be more potent toxicologically than either RDX or HMX, and also has the lowest concentration threshold for soil cleanup. Interestingly, this is not true when accounting for carcinogenic risk, where RDX possesses the highest carcinogenic potency and has the lowest concentration threshold above which soil cleanup would be recommended.

## CONCLUSIONS

The approach just described for deriving risk- and hazard-based concentrations for TNT, RDX, and HMX in soil, above which cleanup would be required or even to which cleanup could be conducted, is scientifically defensible. Equally important is the fact that this approach represents a creative response to the vital challenge of providing risk managers and responsible authorities in the U.S. and other governments worldwide with a tool for systematically selecting strategies for soil cleanup or land use that not only protect public health and safety, but also are timely in their implementation, fiscally practical, and avoid or minimize the loss of valuable limited resources. Given the amount of high explosives to be demilitarized in the future, and the potential magnitude of

HE-contaminated land, this approach is also a proactive measure for addressing the environmental dimension of economic security and regulatory stability.

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Table 1. Concentrations ( $C_i$ s) of high explosives (HEs) in the applicable environmental media (where  $i = a$ , atmospheric gases;  $i = p$ , atmospheric particles;  $i = s$ , soil;  $i = w$ , potable water, and  $i = r$ , surface water) of a 100-km<sup>2</sup> landscape in the central-northeastern ecoregion of the United States (U.S.), assuming a soil-based, steady-state source of contamination. Concentrations of the HEs were predicted using the GEOTOX multimedia transport and transformation computer model<sup>9</sup>, then scaled to a soil concentration of 1.0 mg/kg.

| Energetic compound | Atmospheric gases, $C_a$ (mg/m <sup>3</sup> ) | Atmospheric particles, $C_p$ (mg/m <sup>3</sup> ) | Soil, $C_s$ (mg/kg) | Potable water, $C_w$ (mg/L) | Surface water, $C_r$ (mg/L) |
|--------------------|---|---|---------------------|-----------------------------|-----------------------------|
| TNT                | 0.0 <sup>a</sup>                              | $3.0 \times 10^{-09}$                             | 1.0                 | $4.6 \times 10^{-02}$       | $3.7 \times 10^{-03}$       |
| RDX                | 0.0 <sup>a</sup>                              | $1.1 \times 10^{-10}$                             | 1.0                 | $3.7 \times 10^{-01}$       | $5.9 \times 10^{-02}$       |
| HMX                | 0.0 <sup>a</sup>                              | $3.9 \times 10^{-16}$                             | 1.0                 | $4.4 \times 10^{-01}$       | $4.4 \times 10^{-01}$       |

<sup>a</sup> There is some partitioning of the energetic compound as gases into the atmosphere; however, this fraction is infinitesimally small and therefore considered insignificant.

Table 2. Physicochemical properties of the high explosive (HE) chemicals of interest that are useful for deriving pathway-exposure factors (PEFs).

| Property                                    | Units               | Symbol          | HE and parameter value |                                   |                                   |
|---|---------------------|-----------------|------------------------|-----------------------------------|-----------------------------------|
|   |                     |                 | TNT <sup>a</sup>       | RDX <sup>b</sup>                  | HMX <sup>b</sup>                  |
| Molecular weight                            | g                   | MW              | 227                    | 222                               | 296                               |
| Henry's law constant                        | torr-L/mol          | H               | $2 \times 10^{-3}$     | $5 \times 10^{-6}$                | $1 \times 10^{-10}$               |
| Octanol/water partition coefficient         | dimensionless       | K <sub>ow</sub> | 39.8                   | 7.41 <sup>c</sup>                 | 1.35 <sup>d</sup>                 |
| Diffusion coefficient for air               | m <sup>2</sup> /sec | D <sub>a</sub>  | $5.9 \times 10^{-6}$   | $6.0 \times 10^{-6}$              | $5.1 \times 10^{-6}$              |
| Diffusions coefficient for water            | m <sup>2</sup> /sec | D <sub>l</sub>  | $5.8 \times 10^{-10}$  | $5.9 \times 10^{-10}$             | $5.0 \times 10^{-10}$             |
| Soil/plant partition coefficient (dry mass) | dimensionless       | K <sub>sp</sub> | 6.3 <sup>e</sup>       | 6.3 <sup>e</sup>                  | 3.2 <sup>e</sup>                  |
| Bioconcentration factor in fish             | L/kg                | BCF             | 10.0                   | 5.0                               | 0.5                               |
| Meat/diet biotransfer factor in cattle      | day/kg              | B <sub>t</sub>  | $7.2 \times 10^{-5}$   | $1.9 \times 10^{-7}$ <sup>f</sup> | $3.4 \times 10^{-8}$ <sup>f</sup> |
| Milk/diet biotransfer factor in cattle      | day/L               | B <sub>k</sub>  | $6.5 \times 10^{-6}$   | $5.9 \times 10^{-8}$ <sup>f</sup> | $1.1 \times 10^{-8}$ <sup>f</sup> |

<sup>a</sup> Parameter values are from McKone and Daniels<sup>10</sup>, unless specifically noted.

<sup>b</sup> Parameter values are from Layton et al.<sup>11</sup>, unless specifically noted.

<sup>c</sup> Measurement made by Banerjee et al.<sup>12</sup> (also cited by Layton et al.<sup>11</sup> in Appendix A, Table A-5).

<sup>d</sup> Measurement made by Tucker et al.<sup>13</sup> (also cited by Layton et al.<sup>11</sup> in Appendix A, Table A-5).

<sup>e</sup> Conservative estimate for plant wet weight derived from data presented in Layton et al.<sup>11</sup>.

<sup>f</sup> Biotransfer factors in meat and milk (B<sub>t</sub> and B<sub>k</sub>) estimated using equations developed by Travis and Arms<sup>14</sup> that employ chemical specific values for K<sub>ows</sub> (e.g.,  $\log B_t = \log K_{ow} - 7.6$ ; and  $\log B_k = \log K_{ow} - 8.1$ , where respective K<sub>ows</sub> are from table above).

Table 3. Matrix (from McKone and Daniels<sup>10</sup>) of the algebraic terms and mathematical expressions representing the pathway-exposure factors (PEFs) for deriving doses for TNT, RDX, and HMX in specific environmental media.<sup>a</sup>

| Exposure pathway      | Air (particles),<br>(m <sup>3</sup> /kg•d) | Soil,<br>(kg/kg•d)   | Potable water,<br>(L/kg•d)  | Surface water,<br>(L/kg•d)                        |
|-----------------------|--|--|---|---|
| Inhalation            | F <sub>ph</sub> = 0.31                     | F <sub>sh</sub> = 9.0 × 10 <sup>-9</sup>                                       | F <sub>wh</sub> = 3.2 × 10 <sup>5</sup> ×<br>$\left[ \frac{2.5}{D_l^{0.67}} + \frac{R \times T}{D_a^{0.67} \times H} \right]^{-1}$ <sup>b</sup> |   |
| Ingestion:            |  |  |   |   |
| Water                 |  |  | F <sub>ww</sub> = 0.034   |   |
| Fruits and vegetables | F <sub>pv</sub> = 14                       | F <sub>sv</sub> =<br>1.1 × 10 <sup>-3</sup> × K <sub>sp</sub>                  |   |   |
| Grains                | F <sub>pg</sub> = 22                       | F <sub>sg</sub> =<br>7.9 × 10 <sup>-4</sup> × K <sub>sp</sub>                  |   |   |
| Milk                  | F <sub>pk</sub> = 6600 × B <sub>k</sub>    | F <sub>sk</sub> = [0.0028 +<br>(0.12 × K <sub>sp</sub> )] ×<br>B <sub>k</sub>  | F <sub>wk</sub> = 0.27 × B <sub>k</sub>   |   |
| Meat                  | F <sub>pt</sub> = 2100 × B <sub>t</sub>    | F <sub>st</sub> = [0.0012 +<br>(0.038 × K <sub>sp</sub> )] ×<br>B <sub>t</sub> | F <sub>wt</sub> = 0.14 × B <sub>t</sub>   |   |
| Fish                  |  |  |   | F <sub>ff</sub> = 3.2 ×<br>10 <sup>-4</sup> × BCF |
| Soil                  |  | F <sub>ss</sub> = 1.5 × 10 <sup>-6</sup>                                       |   |   |
| Dermal uptake         |  | F <sub>sd</sub> = 2.6 × 10 <sup>-6</sup>                                       | F <sub>wd</sub> = 0.037   |   |

<sup>a</sup> The subscript abbreviations (ij) associated with each pathway-exposure factor (F<sub>ij</sub>) refer to media, i (i.e., p = particles in air, s = soil, w = potable water, and r = surface water) and route of contact, j (i.e., h = inhalation; w = potable-water ingestion, v = vegetables and fruits ingestion, g = grains ingestion, k = milk ingestion, t = meat ingestion, f = fish ingestion, s = soil ingestion, and d = skin adherence). The product of an F<sub>ij</sub> and a corresponding concentration, C<sub>i</sub> from Table 1, yields the pathway- and media-specific dose [mg/(kg•d)]. The total dose for each HE appears in Table 4 and is the sum of the additions of doses from all media across each exposure pathway [e.g.,  $\sum_i \sum_j F_{ij} \times C_i$ ].

<sup>b</sup> R = universal gas constant, expressed as 62.4 torr-L/(mol•K), and T = temperature expressed as 293 K.

Table 4. Pathway and total doses for TNT, RDX, and HMX. (Computed from products of HE concentrations in Table 1 and applicable PEF equations in Table 3).

| Exposure (E) pathway (j)            | HE-compound, pathway-specific<br>multimedia dose [E <sub>j</sub> ; mg/(kg•d)] |                      |                      |
|-------------------------------------|---|----------------------|----------------------|
|                                     | TNT   | RDX                  | HMX                  |
| Inhalation (h)                      | $5.3 \times 10^{-7}$  | $2.2 \times 10^{-8}$ | $9.0 \times 10^{-9}$ |
| Ingestion, all (g)                  | $1.2 \times 10^{-2}$  | $1.2 \times 10^{-2}$ | $6.1 \times 10^{-3}$ |
| Dermal uptake (d)                   | $1.7 \times 10^{-3}$  | $1.4 \times 10^{-2}$ | $1.6 \times 10^{-2}$ |
| TOTAL ( $\sum E_j = \text{CDI}^a$ ) | $1.4 \times 10^{-2}$  | $2.6 \times 10^{-2}$ | $2.2 \times 10^{-2}$ |

<sup>a</sup> CDI = chronic daily intake over the course of a 70-y lifetime of exposure.

Table 5. Exposure-pathway (j) specific carcinogenic potency (slope<sup>a</sup>) factors (CPF<sub>j</sub>, where j = h for inhalation, g for ingestion, and d for dermal contact) and reference doses (RfDs<sup>b</sup>) for TNT, RDX, and HMX. From data available in the U.S. Environmental Protection Agency's Integrated Risk Information System (IRIS)<sup>15</sup> and Health Effects Assessment Summary Tables (HEAST).<sup>16</sup>

| Factor   | High-explosive (HE) compound      |                                   |                                   |
|--|-----------------------------------|-----------------------------------|-----------------------------------|
|  | TNT                               | RDX                               | HMX                               |
| CPF <sub>h</sub> [risk per mg/(kg•d)]              | Not available                     | Not available                     | Not applicable                    |
| CPF <sub>g</sub> [risk per mg/(kg•d)]              | $3.0 \times 10^{-2}$              | $1.1 \times 10^{-1}$              | Not applicable                    |
| CPF <sub>d</sub> [risk per mg/(kg•d)] <sup>c</sup> | $3.0 \times 10^{-2}$              | $1.1 \times 10^{-1}$              | Not applicable                    |
| RfD [mg/(kg•d)]                                    | $5.0 \times 10^{-4}$ <sup>d</sup> | $3.0 \times 10^{-3}$ <sup>e</sup> | $5.0 \times 10^{-2}$ <sup>f</sup> |

<sup>a</sup> The slope factor is used to estimate the upper-bound probability (the true risk, while not identifiable, is not likely to exceed the upper-bound estimate and in fact may be lower) of an individual developing cancer (carcinogenic potency) at the low dose levels of environmental concern over a 70-y lifetime.<sup>16,17</sup>

<sup>b</sup> RfD is the reference dose representing an estimate (with uncertainty spanning perhaps an order of magnitude or greater) of the daily dose likely to be without appreciable risk of deleterious effects for everyone, including the most sensitive individuals, in the population exposed over a 70-y lifetime.<sup>17</sup> Typically, only oral RfDs are available and by necessity are used for comparison to the CDI<sup>4</sup> (see Table 6).

<sup>c</sup> We assume some similarity of physicochemical behavior for sorption through gut or skin (but not through lung). Accordingly, we use the oral slope factor (CPF<sub>g</sub>) as an estimate of the dermal slope factor (CPF<sub>d</sub>), but do not apply any CPF to inhalation exposure. This procedure, or an even more conservative one is typically performed for assessments of Superfund Sites. In fact, in one remedial investigation we used an even more conservative approach to estimate the cancer risk for those exposure pathways for which slope factors were not available for the chemicals of concern (see Daniels et al.<sup>18</sup>).

<sup>d</sup> Oral RfD for TNT derived from a no observed effect level (NOEL) for critical effects on the liver of beagle dogs.<sup>15</sup>

<sup>e</sup> Oral RfD for RDX derived from a no observed effect level (NOEL) for critical effect of prostate inflammation in male Fischer 344 rats.<sup>15</sup>

<sup>f</sup> Oral RfD for HMX derived from a no observed adverse effect level (NOAEL) for critical effect of hepatic lesions in Fischer 344 rats.<sup>15</sup>

Table 6. Alternative risk- and hazard-based concentrations of TNT, RDX, and HMX in soil for comparison and consideration as levels above which cleanup would be recommended.

| Potentially acceptable levels of risk and the acceptable index for noncarcinogenic hazard | Soil concentration above which cleanup would be recommended $C_{s[\text{cleanup}]_c}$ (mg/kg) |   |  |
|---|---|---|--|
|   | TNT<br>(Group <sup>a</sup> C:<br>possible<br>human<br>carcinogen)                             | RDX<br>(Group <sup>a</sup> C:<br>possible<br>human<br>carcinogen) | HMX<br>(Group <sup>a</sup> D:<br>not classifiable<br>as to human<br>carcinogenicity) |
| $10^{-4}$ excess cancer risk  | $2.4 \times 10^{-1}$  | $3.5 \times 10^{-2}$  | Not applicable   |
| $10^{-6}$ excess cancer risk  | $2.4 \times 10^{-3}$  | $3.5 \times 10^{-4}$  | Not applicable   |
| 1.0 hazard index $\left(\frac{\text{CDI}}{\text{RfD}}\right)$                             | $3.7 \times 10^{-2}$  | $1.2 \times 10^{-1}$  | 2.2  |

<sup>a</sup> U.S. Environmental Protection Agency's weight-of-evidence classification system for expressing the degree to which available data indicate a substance to be a human carcinogen:<sup>17</sup> Group A—substances considered human carcinogens because there is sufficient evidence of carcinogenicity in humans; Group B—substances considered probable human carcinogens because there is either limited evidence of human carcinogenicity (B1) or sufficient evidence of carcinogenicity in animal models to extrapolate to humans, but inadequate or lack of evidence of carcinogenicity in humans (B2); Group C—substances considered possible human carcinogens because of limited evidence of carcinogenicity in animals and inadequate or lack of human data; Group D—substances considered not to be classifiable as human carcinogens because of inadequate or no evidence of carcinogenicity; and Group E—substances for which there is evidence of noncarcinogenicity for humans based on adequate studies revealing no evidence of carcinogenicity.<sup>16</sup>

<sup>b</sup> CDI = chronic daily intake over the course of a 70-y lifetime of exposure; and RfD = reference dose representing an estimate (with uncertainty spanning perhaps an order of magnitude or greater) of the daily dose likely to be without appreciable risk of deleterious effects for everyone, including the most sensitive individuals, in the population exposed over a 70-y lifetime.<sup>17</sup>