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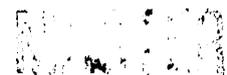
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System Safety Engineering

Date of Issue: June 21, 1993

Draft Paper for submission to:  
Winter Annual Meeting, ASME  
New Orleans, Louisiana  
November 28-December 3, 1993

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U.S. DEPARTMENT OF ENERGY  
under contract DE-AC05-84OR21400



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Analysis of Explosion-induced Releases of Toxic Materials  
at an Environmental Restoration Project

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## ABSTRACT

Prior to 1988, a variety of materials were buried on the US DOE Oak Ridge Reservation. Records of the disposal operations are incomplete and toxic materials may have been placed adjacent to potential explosives. One of the safety concerns in conducting an environmental restoration project at the burial sites, is the possibility of an explosion which could release toxic materials to the atmosphere. A safety analysis examined the consequences of such releases by first postulating an upper bound for the strength of an explosive. A correlation, developed by Steindler and Seefeldt of Argonne National Laboratory, was then used to estimate the amount and particle-size distribution of the material that could become airborne from the explosion. The estimated amount of airborne material was the source term in an atmospheric dispersion model which was used to calculate infinite-time, concentration-time integrals and 5-minute, time-weighted average concentrations at locations down-wind from the explosion. The dispersion model includes particle deposition as a function of particle-size distribution class. The concentration-time integrals and average concentrations were compared to published guidelines to assess the consequences of an accidental explosion.

## INTRODUCTION

Martin Marietta Energy Systems, Inc., has been involved in the environmental restoration of waste sites on the U.S. Department of Energy (DOE) Oak Ridge Reservation. A problem associated with some of these projects is that the potential hazards typically cannot be well characterized; records of the disposal operations are often incomplete so that reliable estimates cannot be made of the kinds and quantities of hazardous materials at the sites.

The first step in analyzing the safety aspects of these projects is to identify those hazards that are known to exist, and rule-out those that cannot be present, on the basis of available information. Additional hazards that might exist are identified on the basis of extrapolating this information using past experience. The potential consequences of these hazards are then analyzed using conservative assumptions and analysis techniques to help compensate for the missing information.

These steps were utilized in analyzing the safety aspects of an environmental restoration project on a former waste burial site on the DOE Reservation. The potential hazards included explosion-induced releases of toxic materials and the analysis indicated the toxicity hazards would determine the safety envelope for conducting the operations.

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<sup>1</sup>Managed by Martin Marietta Energy Systems, Inc. for the U.S. Department of Energy under contract DE-AC05-84OR21400.

## BACKGROUND

The former waste burial site is located near the Oak Ridge Y-12 Plant. The site was first used in 1962 for the disposal of depleted uranium chips (machine turnings), metals, and oxides. A portion of the site (pits) is essentially roads cut into a hillside. Materials for disposal were placed on skids and carefully placed into the dug-out area. The materials were then lightly covered with dirt but not compacted; stacking of materials was common. The pits were first used predominately for the disposal of saw fines of depleted uranium, thorium, and other metals. From 1968 until 1980 the pits were also used for the disposal of acids, bases, and organics. Some of these materials are potential explosives. Packaging of these wastes included drums, cardboard boxes, and metal buckets. Use of the site was discontinued in 1988.

The burial site is being closed in a manner consistent with the Resource Conservation and Recovery Act. This dictates that site run-off/run-on, infiltration to the groundwater, and personnel access to the site be controlled. An impervious cap (Figure 1) will be constructed over the site to control run-off/run-on and infiltration. Because of the explosive nature of some of the buried materials, placement and compaction of fill dirt over the site will be done using armor-plated equipment. No unprotected personnel will be allowed access within 150 m (about 500 ft) of the outer-most edge of the work area during placement of the fill dirt.

## POTENTIAL HAZARDS

A review of the known and assumed conditions at the burial site indicated many potential hazards in the restoration project. Most of these are common to large, earth-moving operations and are controlled through procedures governed by worker-safety laws and industrial standards. Potential hazards which were not common and which required safety analyses were due to the presence of explosive and toxic materials. Although records are incomplete, there are recorded instances of the disposal of potentially-explosive materials (e.g. picric acid, nitrates, and azides). Also, many of the metals can react with water to produce hydrogen which could potentially form pockets of an explosive gas mixture. An upper bound was estimated for the amount of explosive by examining existing records and talking to personnel who were involved in the disposal operations. The largest amount of explosive that could be at any one location appeared to be about 1 lb of picric acid which is equivalent to about 1.08 lb (0.49 kg) TNT. This was the estimated upper bound for the explosive.

The direct effects of an explosion were considered to be injury to operating personnel due to overpressure (blast wave) and shrapnel. No structures are close enough to be affected. Explosive experts from Sandia National Laboratories and the U.S. Army Corps of Engineers (Waterways Experiment Station) were consulted as to the potential range of these direct effects and possible mitigating methods. They indicated that the potential range of direct effects would be small (less than 30 m or about 100 ft from the edge of the site). They recommended that no unprotected personnel be allowed on the site itself but considered the cab of most earth-moving machinery as adequate shielding provided the cab was completely enclosed by a sufficient thickness of high-strength plastic (e.g. 1/2-inch Lexan). The actual operating procedures implement these recommendations and allow for additional conservatism (150 m and armor-plated equipment).

In addition to direct effects, an explosion could release toxic materials to the atmosphere where they could become an inhalation hazard. The most abundant toxic material at the site is

depleted uranium metal in the form of chips and saw fines. Because of this abundance, explosion-induced releases of uranium were analyzed first. As with the explosives, the maximum quantity of uranium at any one location (270 lb) was estimated by examining existing records and talking to personnel who were involved in the disposal operations. A screening process was then used to assess whether any other toxic materials could be a worse toxicity hazard than the uranium.

Assuming equivalent release and dispersion processes, the relative hazard of each material is related to the quantity present and its specific toxicity. The measure of specific toxicity used was the IDLH (NIOSH, 1990) or its equivalent; the lower the IDLH, the greater the specific toxicity. Initially, it was assumed that the maximum quantity of other toxic materials at any one location was less than the quantity of uranium. Therefore, any material with an IDLH greater than that for uranium could not possibly pose a toxicity hazard worse than uranium. On this basis, existing records were searched and any material with an IDLH greater than that for uranium was not considered further. It should be noted that an equivalent IDLH could not be assigned to some materials because they were not well characterized (e.g. solvents) or because no toxicity information could be found in the literature (e.g. decanenitrile). However, most of these materials were present in small quantities and/or could be considered analogous to other materials that had an IDLH greater than that for uranium.

One entry for beryllium indicated the disposal of a quantity (1000 lb) greater than the maximum assumed for uranium. However, personnel who were involved in the disposal operations did not recall the disposal of such a large quantity of beryllium. They thought the entry in the record was incorrect or, more probably, it indicated 1000-lb gross weight of pieces of equipment that was contaminated with small amounts of beryllium. In spite of these uncertainties, the entry was taken at its face value and, due also to the greater specific toxicity (lower equivalent IDLH) for beryllium, an explosion-induced release of beryllium was taken to be the bounding hazard for accident analysis. Benzene, bromine, chloroform, chromic acid, formaldehyde, mercuric chloride, phenol, and trichloroethane were analyzed, in addition to beryllium and uranium, because of the quantity present and/or lower equivalent IDLH.

## ANALYSIS TECHNIQUES

The analysis of explosion-induced releases of toxic materials involve two types of calculations: (1) estimating the amount of toxic material that could become airborne as a result of an explosion and (2) estimating the atmospheric transport of the airborne material to determine the extent of an area where people could be subjected to health effects due to inhaling the material.

Amount of Material Airborne due to an Explosion

A simple correlation is presented by Ayer et. al. (1988, Page 4.49, Equation 4.31) to provide estimates of the amount of material airborne due to an explosion. The correlation can be expressed as

$$\begin{aligned}
 F &= 1.0 && \text{for } M_R < 5 \\
 &= 2.783 M_R^{-0.6383} && \text{for } M_R \geq 5
 \end{aligned} \tag{1}$$

$$M_R = \frac{W_T}{W_E}$$

$F$  is the fraction of material airborne

$M_R$  is the mass ratio

$W_E$  is the strength of the explosive expressed as grams of TNT

$W_T$  is the total weight of material (explosive, material at risk, and any inert material) involved in the explosion, g.

The source for the Ayer et. al. correlation was a paper by Steindler and Seefeldt (1981) of Argonne National Laboratory. In personal discussions with Seefeldt, it was learned that the paper was presented as a "straw man" to encourage further work in this field but, apparently, no further work has been done. They used data, developed by the U.S. Army at Edgewood Arsenal, in order to develop representative curves for the amount and particle size of the material made airborne by an explosion. These data involved the explosion of solids and liquids in a closed chamber of sufficient volume to preclude the build-up of substantial pressure. The chamber was equipped with one or more fans that gently circulated the air within the chamber such that the airborne material was homogenized throughout the chamber volume. The raw data consisted of measured mass concentration and particle-size distribution of the airborne material as a function of time.

The most significant correlating parameter for these data was the mass ratio,  $M_R$ , which varied between 1.0 and 15. Variations due to the type of liquid or solid, state of the solid (cast or degree of compaction), type of explosive, and various geometries were investigated and found to be much less significant. The mass median particle size (particle diameter) increased with  $M_R$  and, at  $M_R$  values greater than 10, the particle-size distribution of the airborne material had two peaks. The particles associated with the larger-diameter peak settled-out very quickly while those associated with the smaller-diameter peak remained airborne long enough to be dispersed. The Steindler and Seefeldt curves are based on an assumed a log-normal distribution of particles around the smaller-diameter peak (using a geometric standard deviation of 2 and the peak particle size as the mean) and represent the upper bound to the data (maximum release fraction).

An expression was developed to fit the Steindler and Seefeldt curve of particle-size versus  $M_R$  (for  $M_R$  values greater than 10) and to be consistent with the Ayer et. al. correlation. This expression is

$$m = 38.962 M_R^{0.3617} \quad (2)$$

The variation of particle size with  $M_R$  is shown in Figure 2.

Since the particle-size of the airborne material is assumed to follow a log-normal distribution with respect to mass, the fraction of material airborne within two particle-size diameters is given by

$$F_R = 0.5 F \left[ \operatorname{erfc} \left( \frac{\ln \left( \frac{d_1}{m} \right)}{\sqrt{2} \ln (g)} \right) - \operatorname{erfc} \left( \frac{\ln \left( \frac{d_2}{m} \right)}{\sqrt{2} \ln (g)} \right) \right] \quad (3)$$

$F_R$  is the fraction of material airborne within particle-size diameters  $d_1$  and  $d_2$

$d_i$  are the particle diameters ( $d_2 > d_1$ ),  $\mu\text{m}$

$m$  is the mass median particle diameter,  $\mu\text{m}$

$g$  is the geometric standard deviation

$\operatorname{erfc}()$  is the complementary error function (Abramowitz and Stegun, 1964, Pages 295 to 329).

Particles sizes (diameters) less than  $10 \mu\text{m}$  are considered to be in the respirable range. The choice of geometric standard deviation has a major effect; increasing the standard deviation increases the fraction of airborne material within the respirable range (Figure 3). Steindler and Seefeldt used a standard deviation of 2 and the Edgewood Arsenal data ranged from 2 to about 3. This analysis conservatively assumed a standard deviation of 4.

#### Atmospheric Transport of Airborne Materials

Atmospheric transport models are used to estimate a time-weighted, average concentration and a concentration-time integral of airborne materials at various locations. These quantities are related by

$$I = \int_0^{\infty} C_i(t) dt \quad (4)$$

$$C = \frac{I}{t_A}$$

$I$  is the infinite-time, concentration-time integral,  $\text{g sec/m}^3$

$C_i$  is the air concentration of the material as a function of time,  $g/m^3$

$C$  is the time-weighted, average concentration of the material,  $g/m^3$

$t_A$  is the averaging time interval, sec.

The averaging time chosen to compare the average concentrations with the equivalent IDLH values is 5 minutes based on discussions with industrial hygienists.

At distances far from the release (greater than about 50 meters), the concentration-time integral is estimated with a dispersion model based on expressions given in Slade (1968, Pages 403 to 404). For an instantaneous release, the concentration-time integral is given by

$$I = \frac{Q}{\pi U \sigma_y \sigma_z} \exp\left(-\frac{H^2}{2 \sigma_z^2}\right) \quad (5)$$

$U$  is the wind speed, m/sec

$\exp()$  is the exponential function,  $e^0$

$\sigma_y$  and  $\sigma_z$  are cross-wind horizontal and vertical dispersion coefficients, respectively, m

$H$  is the height of the release, m.

Hanna et. al. (1982, Pages 67 to 71) present methods to estimate the effect of down-wind deposition of particles. The generally-used method assumes the form

$$C_D = C \exp\left(-\sqrt{\frac{2}{\pi}} \left(\frac{v_D}{U}\right) G\right) \quad (6)$$

$$G = \int_0^x \exp\left(-\frac{H^2}{2 \sigma_z^2}\right) \frac{d x}{\sigma_z}$$

$C_D$  is the air concentration of the material including deposition,  $g/m^3$

$C$  is the air concentration of the material excluding deposition,  $g/m^3$

$v_D$  is a deposition velocity, m/sec

$G$  is an intermediate variable

$x$  is an integration variable

$X$  is the downwind distance, m.

Hanna et. al. (1982, Pages 69 to 71) present values of  $v_D$  as a function of particle size and other factors.

A closed-form approximation for Equation 6 was developed using published correlations for the dispersion coefficients. The correlations used are given by Bloom (1992).

$$\begin{aligned} \sigma_y, \sigma_z &\approx 0.175 \sqrt{X} && \text{for } X \leq X^* \\ &= \frac{a X}{(1.0 + b X)^n} && n = 0, 1/2, 1 \quad \text{for } X > X^* \end{aligned} \quad (7)$$

$X^*$  is the downwind location where the above two expressions are equal, m

a, b, n are empirical coefficients in the expressions recommended by Briggs for constant-rate releases, level ground, and open-country conditions (Hanna et. al., 1982, Table 4.5, Page 30).

The closed-form approximation was developed by substituting Equation 7 into the integral of Equation 6 and expanding the integrand in a Taylor series in  $b_z$  about  $b_z=0$ . Three terms are sufficient for 1 percent accuracy since  $b_z$  is small. The resulting closed-form approximation is

$$\begin{aligned} G &= \frac{2 \sqrt{2} X}{H} S_{NX} [ \exp(-S_{NX}^2) - \sqrt{\pi} S_{NX} \operatorname{erfc}(S_{NX}) ], && \text{for } X \leq X^* \\ G &= \frac{2 \sqrt{2} X^*}{H} S_{NX}^* [ \exp(-S_{NX}^{*2}) - \sqrt{\pi} S_{NX}^* \operatorname{erfc}(S_{NX}^*) ] + 0.5 E_1(S_{FX}^2) \\ &- 0.5 E_1(S_{FX}^{*2}) + \frac{b_z n_z}{a_z} [ X ( \exp(-S_{FX}^2) - 2 \sqrt{\pi} S_{FX} \operatorname{erfc}(S_{FX}) ) \\ &- X^* ( \exp(-S_{FX}^{*2}) - 2 \sqrt{\pi} S_{FX}^* \operatorname{erfc}(S_{FX}^*) ) ] \\ &+ \frac{b_z^2 n_z}{a_z} [ \left( \frac{n_z - 1}{4} + n_z S_{FX}^2 \right) X^2 \exp(-S_{FX}^2) \\ &- \left( \frac{n_z - 1}{4} + n_z S_{FX}^{*2} \right) X^{*2} \exp(-S_{FX}^{*2}) ] \\ &+ \frac{3 b_z^2 n_z (3 n_z - 1) H^2}{8 a_z^3} ( E_1(S_{FX}^2) - E_1(S_{FX}^{*2}) ), && \text{for } X > X^* \end{aligned} \quad (8)$$

$$S_{NX} = \frac{H}{0.175 \sqrt{2} X}, \quad S_{NX}^* = \frac{H}{0.175 \sqrt{2} X^*}$$

$$S_{FX} = \frac{H}{\sqrt{2} a_z X}, \quad S_{FX}^* = \frac{H}{\sqrt{2} a_z X^*}$$
(9)

$E_1(\cdot)$  is the exponential integral function (Abramowitz and Stegun, 1964, Pages 227 to 251).

## RESULTS AND CONCLUSIONS

The analysis techniques were applied to estimating the region where people could be subjected to significant health effects due to inhaling toxic materials. For solids (beryllium and uranium) and non-volatile liquids (solutions of chromic acid and mercuric chloride), only respirable particles (particle sizes less than  $10 \mu\text{m}$ ) were considered. Equations 1, 2, and 3 were applied to estimate the amount airborne and Equations 5 and 6 were used to estimate the maximum downwind extent of the region. A deposition velocity ( $v_D$ ) of 0.01 m/sec was assumed for these particles (Hanna et. al., 1982, Pages 69 to 71). For volatile liquids (benzene, bromine, chloroform, formaldehyde solutions, phenol, and trichloroethane), the amount airborne was estimated using Equation 1 only since all of the liquid was assumed to evaporate. Also, only Equation 5 was used to estimate the downwind extent of the region since no deposition occurs.

The major uncertainty in the above analysis is the application of Equation 1. Confirming data exist only for  $M_R$  in the range of 1 to about 15. Steindler and Seefeldt (1981) extrapolated their correlation to  $M_R = 400$  in their application while this analysis extrapolates the correlation to  $M_R > 1000$ . The amount of inert material to include is also uncertain and two methods were used in this analysis. The operating procedure calls for placing a minimum of 1 ft (about 0.30 m) dirt cover over the buried material before any heavy equipment is to operate on a specific site. This will be done by pushing the dirt ahead of a front-loading bulldozer. Consequently, the depth of the buried explosive was assumed to be 0.30 m. One estimate was based on approximating the crater dimensions resulting from a 0.49 kg TNT charge buried 0.30 m in lightly-compacted dirt. The alternative estimate was smaller and was used in Equation 1. It was based on the fact that the material to be buried was placed on pallets no larger than 4 ft x 4 ft (1.22 x 1.22 m) before being placed in the pits. Therefore, the alternative estimate of the inert material was the weight of the buried material plus the dirt within this 1.22 x 1.22 x 0.30 m volume. The density of loose dirt was assumed to be 2.2 g/ml.

The results are summarized in Table 1. Beryllium represents the worst case and was the determining factor in establishing the extent of the zone beyond which there would be no significant health effects. Formaldehyde was the next worse case because it is very toxic and is present as a volatile liquid solution. Also, the formaldehyde concentration of these solutions was not known and a high value was used to be conservative. In spite of its abundance, uranium was not a significant factor in the analysis.

The maximum distance in Table 1 (300 m) is well within the boundary of the DOE Reservation but just touches a road that is used by some employees to drive to and from the Y-12

Plant. General traffic is not allowed on this road and it is closed during the earth-moving operations. With this restriction, only personnel involved in the project will be within the maximum distance. The project personnel are equipped with respiratory protection and are trained to respond to an explosion.

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Table 1. Summary of Calculated Results

Material of Concern	Concentration* for Negligible Health Effects, mg/m <sup>3</sup>	Distance Beyond Which Negligible Health Effects Occur
Beryllium	0.1	300 m
Depleted Uranium	650 <sup>b</sup>	20 m
Benzene	980	190 m
Bromine	7	100 m
Chloroform	500	70 m
Chromic Acid	3	30 m
Formaldehyde	4	290 m
Mercuric Chloride	1	< 20 m
Phenol	100	170 m
Trichloroethane	280	40 m

a Concentration is generally assumed to be 1/10 of equivalent IDLH.

b Value for uranium is based on a survey of toxicity data (Just and Emler, 1984) and is a concentration-time integral of 650 mg min/m<sup>3</sup>.

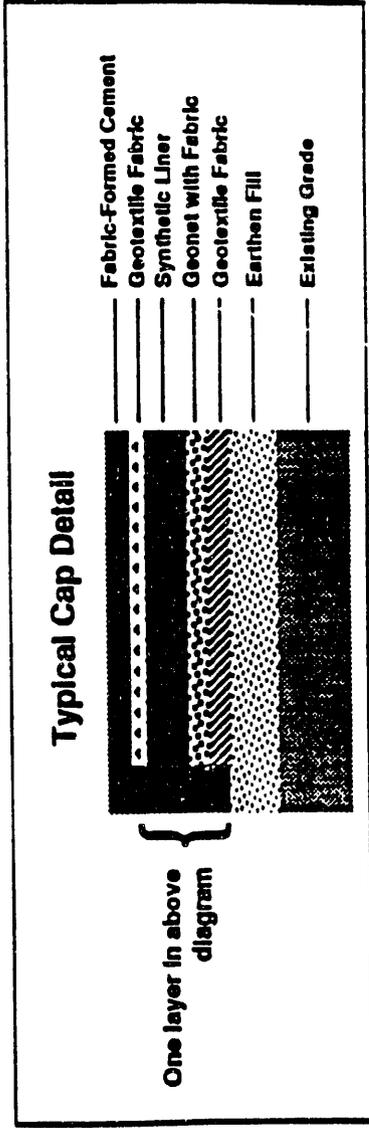
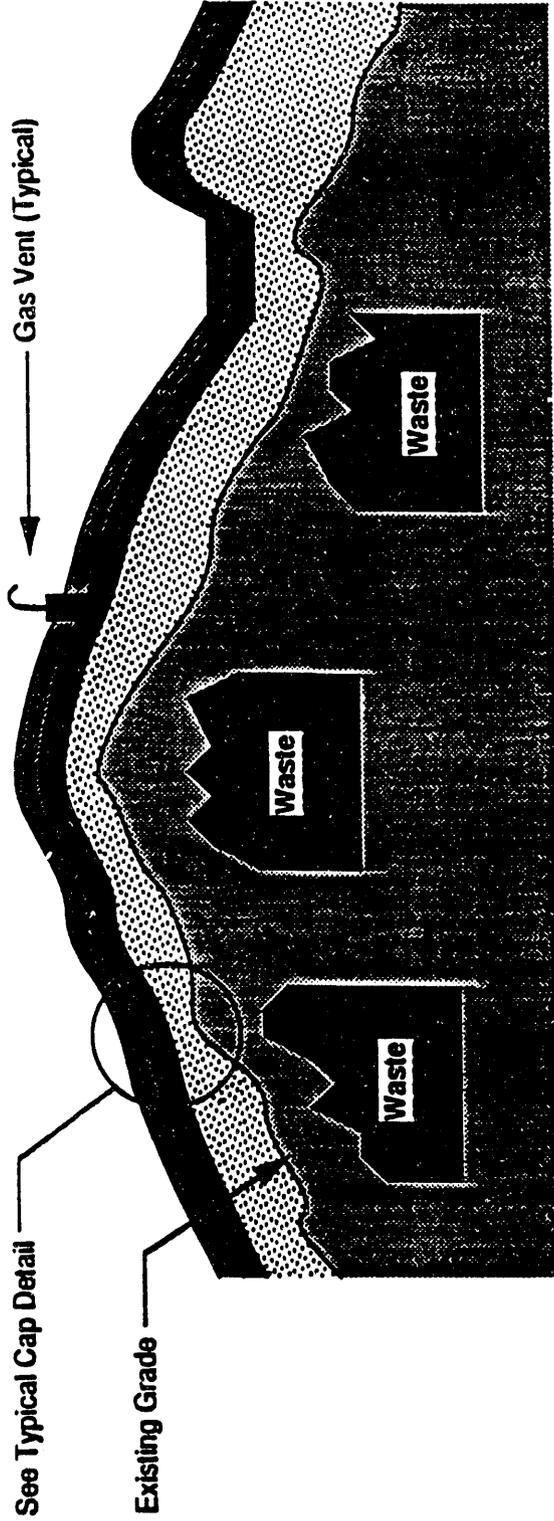
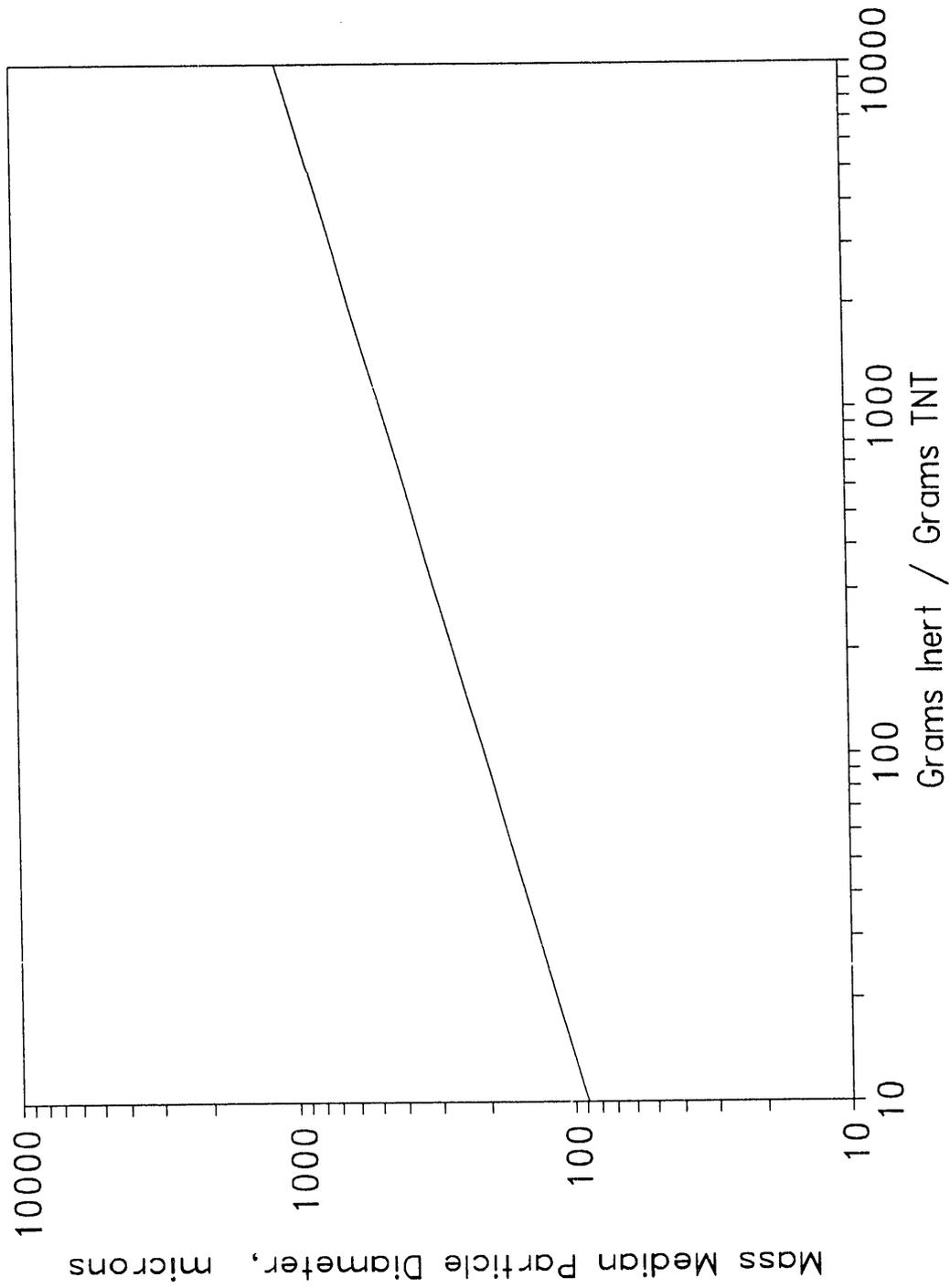


Figure 1. Cross-Section of Waste Burial Site



**Figure 2. Mass Median Particle Diameter versus Mass Ratio**

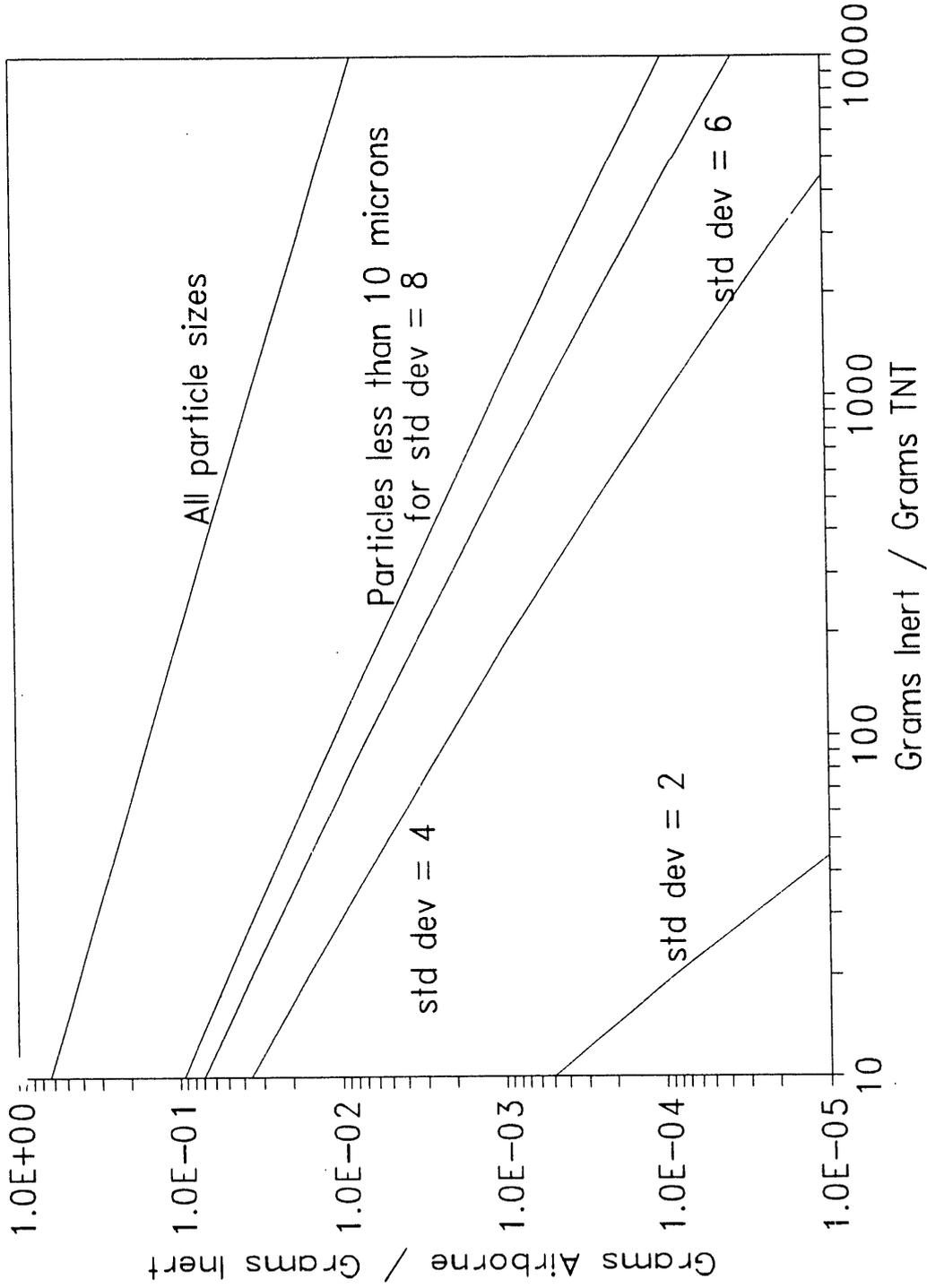


Figure 3. Fraction Airborne versus Mass Ratio

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