OFFICE OF THE
SCIENCE ADVISOR
GUIDANCE

CHAPTER 2

USE OF SOIL
CONCENTRATION DATA IN
EXPOSURE ASSESSMENTS

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ABSTRACT

This is a guidance document for the Department of Toxic Substances Control (DTSC) personnel and Responsible Parties (RPs) in using concentrations of substances in exposure assessments for hazardous waste sites. Specific guidance is provided in evaluation of data quality, interpretation of results, and calculation of source terms for exposure assessment. The use of statistical and spatial sampling data is discussed in the context of the calculation of the source term. Detection limits and the use of negative analytical results are discussed.

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INTRODUCTION

PURPOSE

This is a guidance document for the Department of Toxic Substances Control (DTSC) personnel and Responsible Parties (RPs) in using concentrations of substances in exposure assessments for hazardous waste sites. It is designed to be consistent with the procedures of the U.S. Environmental Protection Agency (EPA) as described in the "Risk Assessment Guidance for Superfund, Human Health Evaluation Manual, Part A, July 1989" (HHEM) Chapters 4 through 6, and provides specific guidance on the procedures related to calculation of exposure point concentrations (EPC) of chemicals.

APPLICATION

The approach described herein is to be used to derive the soil concentration term to be used in the pathway equations which involve direct exposure to soil. It ensures that exposure assessments for hazardous waste sites will incorporate concentration estimates which are adequately protective of the public health and the environment. Estimates of chemical concentrations in soil are to be derived using these principles for all state-lead sites, but issuance of this guidance does not affect exposure assessments in progress or completed before the date of this publication.

LIMITATIONS

This document does not describe in detail the specific statistical methods for sampling, data evaluation, or modeling rate of loss or transport of chemicals at a site. Such

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methods are the subject of other DTSC guidance, and of several scientific publications referenced in this document. It also does not specify how soil concentration data are to be used in models describing pollutant transport, these input data requirements being model-specific.

PRINCIPLE OR THEORY

STATISTICAL SAMPLING

Statistical (random) sampling characterizes, within specified confidence limits or with a specified distribution, the contamination level of a defined unit of soil. Since it is based on probability theory, its validity depends on a lack of bias in sampling.

SPATIAL SAMPLING

Spatial (non-random) sampling characterizes the extent of contamination of soil and is typically used to characterize the spatial extent of the source or the spread of contamination from a source. Spatial sampling does not assume randomness of sampling, and does not characterize a larger unit of a medium. Descriptive statistics such as mean and standard deviation would have little or no meaning when applied to this type of data.

METHODS

DATA REQUIREMENTS.

All samples of environmental media which are intended for use in exposure assessments must be collected, handled, and analyzed properly, according to applicable DTSC and/or EPA guidance.

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Environmental concentrations of chemicals must be estimated based on a limited number of samples, which generally have a wide range of concentrations. Examination of the data can often reveal the underlying sources of the variability, such as time-dependent migration or loss of chemicals. Soil samples used to characterize a hazardous waste site in support of a no-action alternative should be collected using a statistically valid sampling plan, as described by DTSC (1990a). For modeling of the contaminant concentrations in soil, air, and water, spatial distribution may be more appropriate in determining appropriate source terms for the exposure assessment than the statistical methods indicated below, which do not consider spatial distribution.

CALCULATION OF THE SOURCE TERMS.

When a statistically valid sampling plan has been followed, the EPC is ordinarily the lesser of the 95 % upper confidence limit (UCL) of the arithmetic mean of the sample values, or the maximum observed value. If a probabilistic approach is being used, concentration data are entered as a distribution. When concentrations are predicted through a distribution or dispersion model, the UCL is used in the exposure assessment. Statistical methods for analyzing log-normal distributions are described in Gilbert (1987), Parkin et al. (1988), and in a draft DTSC standard (DTSC, 1990b).

Point Sources

A chemical in soil or ground water often appears to be spreading out from a point source along a gradient. These data are well suited to a model which considers spatial distribution, and can effectively characterize contamination prior to remediation. If one chooses to apply summary statistics, it will often be appropriate to divide the site into multiple area sources instead of considering the entire site as a single source; area-weighted averaging of areas of high and low concentrations of a chemical introduces less error than averaging across the whole site, and can compensate for oversampling of heavily contaminated areas.

Statistical Validity

The statistical validity of the sampling plan is critical if a no-action alternative is proposed. For a remediation feasibility study, it is more important to

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characterize the extent of contamination than to assure that the samples are representative of the entire site.

Residential-use Scenarios

For residential land-use scenarios, the site-wide average concentration is less important than the maximum concentration in potential back-yard-sized areas. An appropriate-sized area for averaging sample values is 1000 ft^2, as discussed in Hadley and Sedman (1990). (The recommendation in this article to use average chemical concentrations in soil in exposure assessments is superseded by the current use of the UCL.) Surface samples or depth-weighted average concentrations down to 10 feet below the surface, whichever is greater, should be used in exposure calculations.

USE OF NEGATIVE ANALYTICAL RESULTS

Every analytical technique used to measure the concentrations of chemicals has associated limits of detection (LOD) and limits of quantitation (LOQ). A chemical that is not detected in a sample is below the LOD. A chemical that is detected but in such low amounts that its concentration cannot be accurately determined is below the LOQ. These limits vary 1) among different laboratories, 2) within a given laboratory depending on instrument maintenance, 3) among samples depending on the concentration of interfering chemicals, and 4) depending on the characteristics of the sample matrix. When a chemical is reported as not detected in a sample, the actual concentration is any value up to the LOD. When the chemical has been found in some of the samples and is not clearly spatially limited, it is assumed to exist in samples in which it was not detected (ND). The assignment of a value of one-half the LOD to all samples reported as "ND" reflects the assumption that the samples are equally likely to have any value up to the detection limit. Similarly, when the analyte is detected but not quantifiable, a value midway between the LOD and the LOQ should be assigned. If only the LOQ is reported, negative results are assumed to be from zero to the LOQ, and are assigned a value of one-half the LOQ. When the sample values above the LOQ level are log-normally distributed, it is reasonable to presume that values below the LOQ are also log-normally distributed, and the reported detection limit divided by the square root of two (1.414) should be assigned as a proxy value for negative analytical results (Hartung and Reed, 1987 and EPA, 1988).

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Very High LODs or LOQs

In some cases the limit of detection or quantitation of a specific chemical in a sample will be very high due to an interfering matrix of substances. The best approach to these results is to re-analyze the samples using additional sample preparation and/or more sensitive analytical procedures. However, the distortion of the calculated value of the source term by these high detection limits is limited, because if the UCL exceeds the maximum detected value, the latter is used as the source term.

When Chemical is Limited in Distribution

When the spatial or temporal distribution of a chemical has been adequately characterized, and it is clear that the distribution of a chemical is limited in time and/or space (e.g. derived from a specific spill or source, with inadequate time to spread across the site), negative results from locations distant from where the chemical has been found may be presumed to be zero. However, the samples from uncontaminated areas should not be averaged with those from contaminated areas.

CORRECTION FOR BACKGROUND

Many substances, such as metals in soil, or nitrate in water, can be found in all samples. For these analytes it is necessary to determine what fraction of the concentrations found, if any, is due to the hazardous waste site, and what fraction represents background. "Background" refers to the average concentration of the chemical(s) in similar, nearby areas which have not been specifically contaminated and may be highly variable. It could be necessary to analyze many samples from areas near the site to adequately characterize the background. The statistics for such samples should be handled the same as for site-derived chemicals. Values that seem unreasonably high or low should be questioned, because this may indicate a methodological problem. Values obtained at other sites and by other agencies can provide worthwhile perspective. The background values are used differently, depending on whether the substance is presumed to act via a non-threshold or threshold mechanism of toxicity.

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Substances Acting via non-Threshold Mechanisms

Background, pre-existing contamination does not alter the risk posed by non-threshold agents (carcinogens) associated with a waste site, calculated by the standard linear low-dose extrapolation methods. Because the Responsible Party is not obligated to clean up the background environmental concentrations of potentially toxic substances, it is reasonable to subtract such background concentrations from the measured levels.

Substances Acting via Threshold Mechanisms

For substances which have a threshold of action, the background level plus the concentration of chemical from a waste site might produce a combined exposure which exceeds the threshold for toxic effects. Subtracting the background levels before calculating risk could therefore misrepresent the threat to public health associated with the site-related contamination, resulting in the false conclusion that the site-related chemicals do not impose a risk of adverse effects on health. This should not, however, be construed as implying that the Responsible Party would be obligated to clean up the background contamination. Background levels would be considered later, as part of risk management.
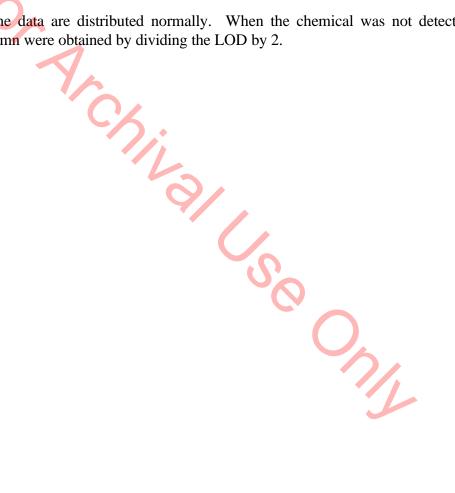
SAMPLE CALCULATION

The LOD of a chemical can vary in different samples of the same medium if one chemical interferes with the analysis of another. In the following example the effect of co-contamination with toluene on xylene quantitation limits is illustrated, and the effect of these LODs on the estimated chemical concentration is shown.

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	Toluene conc.	Xylene conc.	Xylene LOD	Assumed Xylene conc.[1]	Assumed Xylene conc.[2]
Sample 1	1,000	ND	10	7.1	5
Sample 2	20,000	ND	200	141	100
Sample 3	10,000	ND	200	141	100
Sample 4	30,000	500	400	500	500
Mean				197	176
UCL				446	436

[1] Assuming that the data are distributed log-normally. When the chemical was not detected, the values in this column were obtained by dividing the LOD by 1.4.

[2] Assuming that the data are distributed normally. When the chemical was not detected, the values in this column were obtained by dividing the LOD by 2.

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