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Standard Guide for
Determination of Representative Sediment Background Concentrations[1]

This standard is issued under the fixed designation E3242; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon (ε) indicates an editorial change since the last revision or reapproval.

1. Scope

1.1 This guide focuses on the approach for determination of representative sediment background concentrations used for remedial actions performed under various regulatory programs, including the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA). Although many of the references cited in this guide are CERCLA oriented, the guide is applicable to remedial actions performed under local, state, federal, and international cleanup programs. However, the guide does not describe requirements for each jurisdiction. The requirements for the regulatory entity under which the cleanup is performed should be reviewed to confirm compliance.

1.2 This guide provides a framework, including specific statistical and geochemical considerations, as well as case studies, demonstrating the approach to determine representative sediment background concentrations. This guide is intended to inform, complement, and support, but not supersede, local, state, federal, or international regulations.

1.2.1 This guide does not address methods and means of data collection (Guide E3163, Guide E3164.)

1.2.2 This guide is designed to apply to contaminated sediment sites where sediment data have been collected and are readily available. Additionally, this guide assumes that risk assessments have been performed, so that the contaminants/chemicals of interest that exceed risk-based thresholds have been identified.

1.2.3 Furthermore, this guide presumes that risk-based thresholds identified are low enough to pose corrective action implementation challenges, and/or the site is subject to recontamination from ongoing anthropogenic and/or natural sources that are not controlled. In both cases, representative sediment background concentrations will be useful for determining the extent of corrective remedial actions (when used as remedial goals), evaluating risks posed by representative background concentrations, and establishing appropriate post-remedial monitoring plans.

1.3 *Units*—The values stated in SI units are to be regarded as standard. No other units of measurement are included in this standard.

1.4 *This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the responsibility of the user of this standard to establish appropriate safety, health, and environmental practices and determine the applicability of regulatory limitations prior to use.*

1.5 *This international standard was developed in accordance with internationally recognized principles on standardization established in the Decision on Principles for the Development of International Standards, Guides and Recommendations issued by the World Trade Organization Technical Barriers to Trade (TBT) Committee.*

2. Referenced Documents

2.1 *ASTM Standards:*[2]

D6312 Guide for Developing Appropriate Statistical Approaches for Groundwater Detection Monitoring Programs at Waste Disposal Facilities

D7048 Guide for Applying Statistical Methods for Assessment and Corrective Action Environmental Monitoring Programs

E178 Practice for Dealing With Outlying Observations

E1689 Guide for Developing Conceptual Site Models for Contaminated Sites

E3163 Guide for Selection and Application of Analytical Methods and Procedures Used during Sediment Corrective Action

E3164 Guide for Sediment Corrective Action – Monitoring

3. Terminology

3.1 *Definitions:*

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[2] For referenced ASTM standards, visit the ASTM website, www.astm.org, or contact ASTM Customer Service at service@astm.org. For *Annual Book of ASTM Standards* volume information, refer to the standard's Document Summary page on the ASTM website.

3.1.1 *anthropogenic background, n*—natural and human-made substances present in the environment as a result of human activities, not specifically related to the site release in question. (**1**)[3]

3.1.2 *arithmetic mean, n*—a measure of central tendency that is the sum of observed values in the sample divided by the sample size.

3.1.3 *distribution, n*—in statistics, a set of all values that individual observations may acquire and the frequency of their occurrence in the sample or population.

3.1.4 *false negative error, n*—also known as "Type II" error. For the purposes of this guide, in site versus background comparisons, the error that occurs when the statistical procedure does not indicate concentrations above background, when such concentrations are present.

3.1.5 *false outlier, n*—measurements that are very large or small relative to the rest of the data, but represent true extreme values of a distribution and indicate more variability in the population than was expected. (**2**)

3.1.6 *false positive error, n*—also known as "Type I" error. For the purposes of this guide, in site versus background comparisons, the error that occurs when the statistical procedure indicates concentrations above background, when such concentrations are not present.

3.1.7 *high nondetect, n*—a nondetect concentration that resides in the upper decile of the analyte's distribution (that is, above the 90th percentile of the data set).

3.1.8 *median, n*—in statistics, the value below which 50 % of a sample or population falls.

3.1.9 *nonparametric, adj*—a term referring to a statistical technique in which the distribution of the constituent in the population is unknown and is not restricted to be of a specified form (Guide D7048).

3.1.10 *outlier, n*—see *outlying observation*.

3.1.11 *outlying observation, n*—an extreme observation in either direction that appears to deviate markedly in value from other members of the sample in which it appears (Practice E178).

3.1.12 *parametric, adj*—a term referring to a statistical technique in which the distribution of the constituent in the population is assumed to be known (Guide D7048)

3.1.13 *probability plot, n*—a plot of ascending observations in a sample, versus their corresponding cumulative probabilities, based on a specified distribution function.

3.1.14 *representative background concentrations, n*—a chemical concentration that is inclusive of naturally occurring sources and anthropogenic sources, similar to those present at a site, but not related to site releases and site-related activities (Guide E3164).

3.1.15 *sample, n*—in statistics, a group of observations taken from a population that serve to provide information that may be used as a basis for making a decision concerning the population.

3.1.16 *sample size, n*—in statistics, the number of observations or measurements in the sample.

3.1.17 *sediment(s), n*—a matrix of pore water and particles including gravel, sand, silt, clay and other natural and anthropogenic substances that have settled at the bottom of a tidal or nontidal body of water (Guide E3163).

3.1.18 *significance, n*—in statistical hypothesis testing, the probability of the test rejecting the null hypothesis, when the null hypothesis is actually true.

3.1.19 *tolerable error rate, n*—the specified maximum acceptable error rate set by the decision maker.

3.1.20 *true outlier, n*—measurements that are very large or small relative to the rest of the data, but are a result of transcription errors, data-coding errors, or measurement system problems. (**2**)

3.1.21 *upper confidence limit (UCL), n*—an upper limit of an estimated value, such as the mean, that has a specified probability of including the true value, with a specified confidence level.

3.1.22 *upper percentile, n*—the value below which a specified percentage of observed values falls.

3.1.23 *upper prediction limit (UPL), n*—the value below which a specified number of future independent measurements will fall, with a specified confidence level.

3.1.24 *upper tolerance limit (UTL), n*—the value below which a specified percentage of observed values falls, with a specified confidence level.

3.2 *Definitions of Terms Specific to This Standard:*

3.2.1 *background reference areas, n*—for the purposes of this guide, sediment areas that have similar physical, chemical, geological, biological, and land-use characteristics as the site being investigated, but are not affected by site-related releases and/or activities.

3.2.2 *background threshold value (BTV), n*—for the purposes of this guide, a measure of the upper limit of representative background concentrations.

3.2.3 *cleanup level, n*—for the purposes of this guide, the prescribed average or point sediment concentration of a chemical that shall not be exceeded at the remediated site.

3.2.4 *conceptual site model (CSM), n*—for the purposes of this guide, the integrated representation of the physical and environmental context, the complete and potentially complete exposure pathways and the potential fate and transport of potential contaminants of concern at a site.

3.2.4.1 *Discussion*—The CSM should include both the current understanding of the site and an understanding of the potential future conditions and uses for the site. It provides a method to conduct the exposure pathway evaluation, inventory the exposure pathways evaluated, and determine the status of the exposure pathways as incomplete, potentially complete, or complete.

3.2.5 *population, n*—for the purposes of this guide, in statistics, a comprehensive set of values consisting of all possible observations or measurements of a certain phenomenon from which a sample is to be drawn.

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[3] The boldface numbers in parentheses refer to a list of references at the end of this standard.

3.2.6 *potential contaminant of concern (PCOC), n*—for the purposes of this guide, a contaminant whose sediment concentrations at the site may exceed applicable screening levels; this includes chemicals of potential environmental concern (COPECs) and chemicals of potential concern (COPCs).

3.2.7 *reference element, n*—for the purposes of this guide, a major element that represents the mineral to which a trace element may be adsorbed.

3.2.8 *trace element, n*—for the purposes of this guide, an element defined as generally being present at less than 0.1 weight percent in the sediment sample; its natural concentrations are typically one or more orders of magnitude lower than those of the reference elements.

4. Significance and Use

4.1 *Intended Use:* This guide may be used by various parties involved in sediment corrective action programs, including regulatory agencies, project sponsors, environmental consultants, toxicologists, risk assessors, site remediation professionals, environmental contractors, and other stakeholders.

4.2 *Related ASTM Standards:* This guide is related to Guide E3164, which addresses corrective action monitoring before, during, and after sediment remediation activities; as well as Guide E3163, concerning sediment analytical techniques used during sediment programs.

4.3 *Use of Representative Background to Set a Boundary:* Representative background concentrations for sediments can be used to delineate a sediment corrective action, establishing the boundary of the sediment corrective action by distinguishing site-related impacts from representative background concentrations.

4.4 *Use of Representative Background to Establish Cleanup Levels:* Representative background concentrations for sediments can also be used to establish cleanup levels for use in sediment corrective actions. In cases where risk-based sediment cleanup levels are below representative background concentrations, background concentrations are typically used as the cleanup level. This ensures that the cleanup levels are sustainable. Any recontamination from ongoing sources will eventually result in surface sediment concentrations greater than the risk-based cleanup level, but the surface sediment should still meet a cleanup level based on representative background concentrations, even after recontamination.

4.5 *Use of Representative Background in Risk Assessments:* Representative background concentrations can be used in the risk assessment process (including human and ecological risk assessments) to understand risks posed by background levels of contaminants to human health and the environment, and the incremental risks posed by site-related releases and/or activities that result in sediment concentrations that exceed representative background concentrations. Conversely, they can be used to estimate the risk reduction for various contaminants, if sediment is remediated from existing PCOC concentrations to lower values (that is, representative background concentrations).

4.6 *Use of Representative Background in Long-Term Monitoring Programs:* Long-term monitoring programs can also use representative background concentrations in sediment, either as a corrective action target or to understand how post-corrective action concentrations compare to sources not attributable to site releases and/or activities. Typically, source control actions taken to ensure that site-related releases are controlled and will not re-contaminate the post-corrective action sediments must be developed based on an understanding of ongoing contributions from representative background. Ongoing sources not related to site-related releases and/or activities (that may or may not be subject to source control actions) must be considered in this evaluation.

4.7 *Importance of the CSM:* The users of this guide are encouraged to continuously update and refine the CSM used to describe the physical properties, chemical composition and occurrence, biologic features, and environmental conditions of the sediment corrective action project (Guide E1689).

4.8 *Reference Material:* This guide should be used in conjunction with other reference material (refer to Section 2 and References at the end of this guide) to direct the user in developing and implementing sediment corrective action programs.

4.9 *Flexible Site-Specific Implementation:* This guide provides a systematic, but flexible, framework to accommodate variations in approaches by regulatory agencies and by the user based on project objectives, site complexity, unique site features, regulatory requirements, newly developed guidance, newly published scientific research, changes in regulatory criteria, advances in scientific knowledge and technical capability, and unforeseen circumstances.

4.10 *Systematic Project Planning and Scoping Process:* When applying this guide, the user should undertake a systematic project planning and scoping process to collect information to assist in making site-specific, user-defined decisions for a particular project, including assembling an experienced team of project professionals (that is, experienced practitioners familiar with current sediment site characterization and remediation techniques, as well as geochemistry, and statistics). These practitioners should have the appropriate expertise to scope, plan, and execute a sediment data acquisition and analysis program. This team may include, but is not limited to, project sponsors, environmental consultants, toxicologists, site remediation professionals, analytical chemists, geochemists, and statisticians.

5. Importance of Representative Background

5.1 At many sediment sites, multiple sources may contribute to the nature and extent of contamination. The largest contribution of contamination at sediment sites is typically attributed to site releases and/or activities. However, contamination can also result from natural and ongoing anthropogenic sources not related to site releases and/or activities. Discharges from combined sewer overflows (CSOs), industrial outfalls, surface runoff, and/or storm sewer systems (municipal and private) are examples of ongoing anthropogenic sources that may be unrelated to site releases and/or activities.

5.2 The off-site contamination not associated with site releases and/or activities is considered a component of representative background concentrations and will continue to be a source of contamination to the site, unless all transport pathways are eliminated. A primary objective of determining representative background concentrations is to account for any background chemical input (both natural and anthropogenic) that is expected to continue migrating onto the site. It is recognized that one of the important principles for management of contaminated sediment sites is the control of sources of contamination, to the greatest extent practicable, prior to the initiation of corrective actions at the subject site (for example, see (**3, 4**)). However, it is rarely practicable to control all background sources.

5.3 Technically defensible representative background concentrations are those that accurately reflect chemical inputs to a site from natural and ongoing anthropogenic sources unrelated to site releases and/or activities. In addition to informing or establishing cleanup levels, representative background concentrations can assist in determining site boundaries, identifying PCOCs, establishing and optimizing realistic long-term monitoring plans, and assessing the performance of corrective actions.

5.4 In the absence of representative background concentrations, risk-based cleanup levels may be used inappropriately at sites where representative background concentrations are actually greater than the risk-based cleanup levels. Similarly, if the representative background concentrations have been erroneously calculated (for example, by the inappropriate exclusion of some outlier data points [false outliers], refer to Section 11), inappropriately low cleanup goals could be used in the corrective action evaluation process. Under both circumstances, sites will eventually return to representative background concentrations after corrective actions are completed and cleanup goals will be exceeded. Due to exceedances of the inappropriately low cleanup goals, the corrective actions would be perceived as failures.

5.5 Attempting to implement corrective actions to achieve concentrations less than representative background is not sustainable over the long-term and can require considerable expenditures that serve no environmental or public health purpose. The process described in this guide (refer to Section 6) is intended to help promote a scientifically sound approach for establishing representative background concentrations, leading to corrective action decisions that avoid costly perceived corrective action failures at sediment sites.

6. Overview of the Process

6.1 As shown in Fig. 1, to determine representative background concentrations, a thorough understanding of a site is necessary. This can be accomplished by developing a CSM (see Guide E3164, Appendix X2) that informs the selection of the background reference area(s) where data collection will occur. Additionally, the site PCOCs must be identified.

6.2 Representative background concentrations are typically derived in two ways: *(1)* collecting sediment samples in background reference areas that have characteristics as similar as possible to that of the site (based on a preliminary CSM for the site), and/or *(2)* extracting representative background concentrations from the site data from portions of the site that have been unaffected by site releases and/or activities. Additionally, under certain circumstances *(1)* and *(2)* can be combined to derive representative background concentrations. Sections 8 and 9 provide additional information concerning the collection and extraction of representative background concentrations. Appendix X1 provides a simple case study illustrating the selection of representative background areas.

6.3 Once the preliminary CSM has been developed, background reference area(s) can be identified for sampling (refer to Section 8).

6.4 When analytical data are available—either by collecting new data or by extricating data from the existing site data set—data can be visualized with a variety of techniques. Section 10 describes several types of graphical methods that aid in statistical and geochemical evaluations of the data.

6.5 Evaluation of outliers is performed to identify statistical outlying observations in the candidate background data set, as further discussed in Section 11.

6.6 Chemical and geochemical processes that influence the concentrations of elements in sediment are also considered when identifying a representative background data set, evaluating statistical outliers, and comparing analyses of site versus background samples. The use of geochemical evaluation is discussed in Sections 7 and 12.

6.7 As described in Section 13, the identification of representative background data should include the screening of high-nondetect values, outlier testing, consideration of impacts from organic contaminants, and geochemical evaluation of metals concentrations.

6.8 As described in Section 14, once a technically sound background data set has been obtained, representative background concentration values can be calculated by a number of methods and applied for a variety of uses.

7. Chemical and Geochemical Considerations

7.1 Identifying representative sediment background concentrations, to include in a background data set, is typically an iterative process. The goal is to maximize the likelihood of obtaining a final data set that contains a wide range of representative background concentrations and that captures the natural and anthropogenic variance in the data set, without biasing the data by including "true outliers" (3.1.20 and 11.4), excluding "false outliers" (3.1.5 and 11.4), or including "high-nondetect" values (3.1.7 and 13.1.1) in the background data set. The resulting background data set is less likely to yield erroneous conclusions when used for statistical and geochemical comparisons to site data. The analytes that are the focus of the background study should be understood and evaluated with respect to their source(s) and potential site-related impacts. The screening steps of 13.1 include consideration of geochemistry, as well as consideration of other characteristics of the candidate background samples, such as laboratory reporting limits and qualifiers.

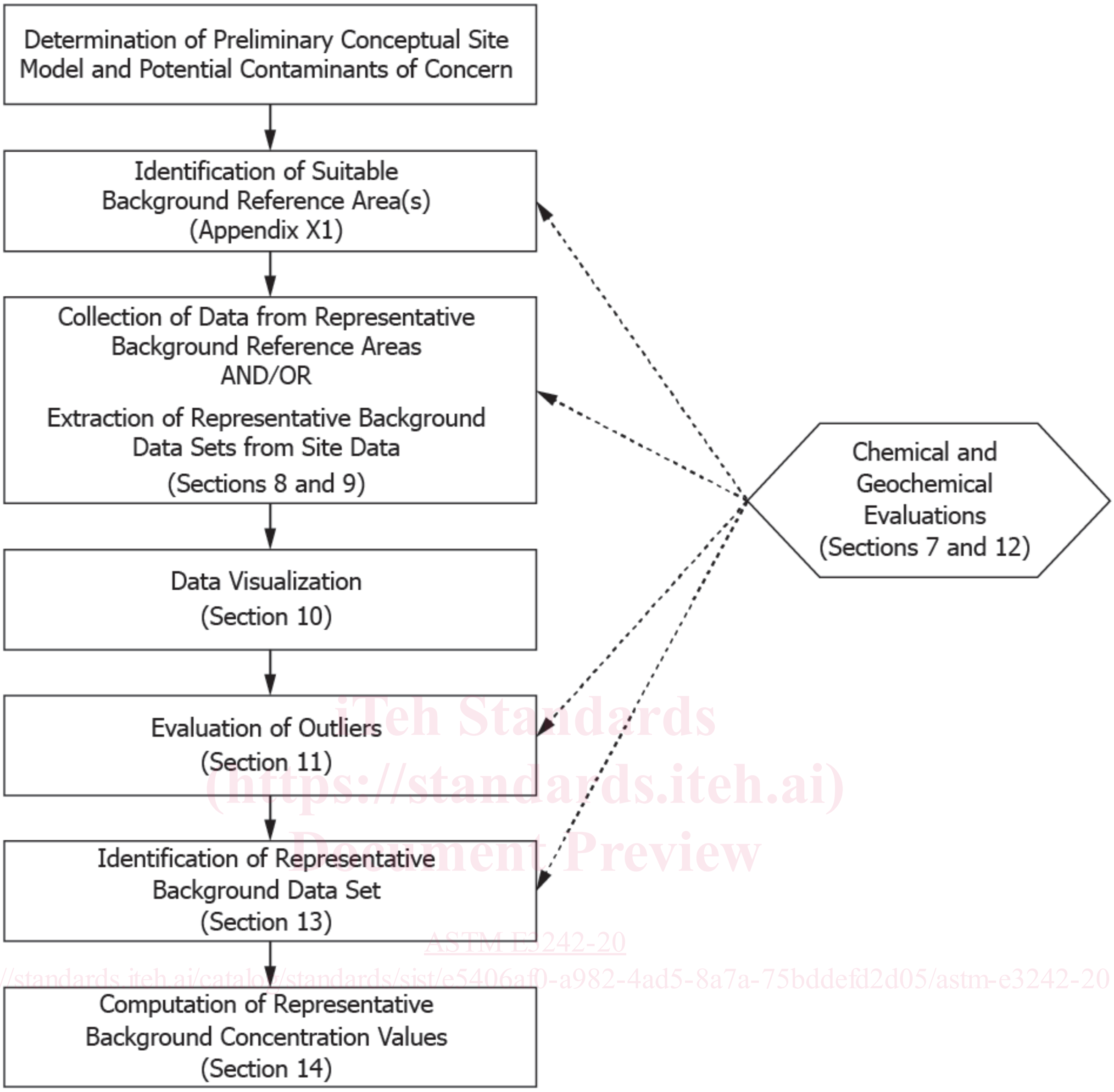

FIG. 1 Overview of the Process

7.2 *Organic Compounds:*

7.2.1 Background studies may focus on one or more groups of organic compounds that can be pervasive in the environment, typically at low concentrations. They include polycyclic aromatic hydrocarbons (PAHs) and polychlorinated dibenzo-*p*-dioxins and dibenzofurans (PCDD/F), which can have both natural and anthropogenic sources; and pesticides and polychlorinated biphenyls (PCBs), which are solely from anthropogenic sources (**5**, **6**, **7**).

7.2.2 Different sources of PAHs have different proportions of individual PAH compounds. These proportions provide a signature, or "fingerprint," that can be used to examine the PAH data on a sample-by-sample basis. Selected PAH compound ratios (for example, fluoranthene/pyrene) reflect the thermal stability of related isomers, and they can be examined to distinguish pyrogenic and petrogenic sources, among other forensic uses (Appendix X2; also see Appendix A of (**8**)). Normalized ratios (for example, anthracene/[anthracene+phenanthrene]), visualized using double-ratio plots, can be a powerful technique for PAH data evaluation (**9**).

7.2.3 PAH, PCB, and PCDD/F data are well suited for evaluation using the "FALCON" fingerprinting approach described in (**10**). FALCON is a simple method that is suitable for limited data sets; more sophisticated (but more complicated) methods for exploratory data analysis of organic compounds can also be used. For example, multi-component mixtures are amenable to compositional analysis via a number of different multivariate data analysis techniques (**5**, **11**). All of these methods allow the investigator to identify samples that have ratios or fingerprints that differ from those of other samples and that might not represent ambient background conditions. For example, a background sediment sample that possesses relatively high PAH concentrations that also exhibits PAH ratios identical to those of the other background sediment samples may be part of the background population(s) and should be retained in the background data set. In contrast, if this sample exhibits distinctly different PAH ratios relative to those of the other background sediment samples, then it warrants further investigation and possible exclusion from the representative background data set.

7.3 *Inorganics:*

7.3.1 *Naturally Occurring Elements*—Background studies commonly focus on the concentrations of elements, due to their ubiquity in nature and the fact that naturally occurring concentrations often exceed risk-based screening values. Naturally occurring elements detected in sediment derive from parent material (commonly bedrock) that was chemically and physically weathered and then transported from other locations to a point of deposition. Climate and the composition of the parent material determine the minerals that form during sediment development. Some minerals, such as metal sulfides, can precipitate from the sediment pore water, and this contributes to the detected sediment concentrations.

7.3.1.1 Common reference elements in sediment include aluminum, calcium, iron, magnesium, and manganese. These elements are found at higher concentrations in sediments (often greater than 1 weight percent) and serve as potential reference elements during geochemical evaluations (Section 12). Trace elements are typically defined as being present at less than 0.1 weight percent, and their natural concentrations can be one or more orders of magnitude lower than those of the reference elements. The USEPA's Target Analyte List (TAL) of 23 metals includes most of the trace elements that may be of interest at most sediment sites: antimony, arsenic, barium, beryllium, cadmium, chromium, cobalt, copper, lead, mercury, nickel, selenium, silver, thallium, vanadium, and zinc. Molybdenum and tin are other trace elements that are not included in the USEPA's TAL, but are potential contaminants of concern at some sediment sites and may need to be analyzed.

7.3.2 *Anthropogenic Input of Elements*—Inorganic contaminants can have many different sources; see references such as (**5, 12**). During a sediment background study, it is important to identify and exclude any samples that have been impacted by site releases and/or activities. For example, the addition of a trace element, such as zinc, from a contaminant source at a given location will result in an elevated trace-versus-reference element ratio in the sample relative to unimpacted samples. This is because the trace element was added to the sediment at that sample location but the reference element was not added (that is, the trace element concentration has increased while the reference element concentration is unchanged). Therefore, geochemical evaluation of all candidate background samples is recommended, to identify potentially impacted samples and flag them for removal, when appropriate. Section 12 provides an overview of the theory behind geochemical evaluation, and the case studies in Appendix X3 provide detailed examples of geochemical evaluation using a variety of sediment data sets.

8. Collection of Data from Representative Background Reference Areas

8.1 The background reference area(s) should have similar physical, chemical, geological, biological, and land-use characteristics as the site. Additionally, such areas should not be influenced by site-related releases and/or activities, but should include ongoing sources similar to those present at the site, as well as a similar land use (Guide E3164). For example, if the subject site is in an industrial area with CSOs, the background reference area(s) should be in an industrial area with CSOs (refer to Appendix X1).

8.2 The more developed the CSM, the more informed the choice of background reference areas will be. Additional information is provided in Guide E3164 and (**13**).

8.3 Once the background reference area(s) are identified, data collection can occur. This guide does not address methods and means of data collection. The optimal number of background reference area sediment samples needs to be determined on a project-specific basis by qualified personnel on the project team (4.10 and 14.2).

8.4 Representative background concentrations may be characteristic of one or more statistical populations with distinct features. For example, sediment background concentrations from a basin surrounded by urban developments and/or industrial areas are distinctly different from those collected from another portion of the same basin surrounded by agricultural areas (refer to Appendix X1). Combining background data sets that represent different statistical populations can lead to erroneous or misleading results. Representative background concentrations are those that are collected from sampling locations (either background reference areas or areas within the site that are unimpacted by site releases and/or activities) with physical, chemical, geological, biological, and land-use characteristics similar to the site.

9. Extraction of Representative Background Data Sets from Site Data

9.1 Although collecting samples from off-site representative background reference areas is typically preferable, in many instances (especially in urban areas), identification of such areas are problematic. Under such conditions, representative background data sets may potentially be extracted from site data, as long as part of the site has not been impacted by site releases and/or activities. Even when data from separate off-site background reference areas are available, an extracted site-specific background data set provides an additional line of evidence when determining representative background concentrations. Therefore, an analysis of existing site data is always recommended. A more complete review of this topic is presented in (**14**).

9.2 Extracting representative background concentrations from site data not only maximizes the utility of existing data, but also avoids the often complex task of selecting separate background reference areas that adequately display physical, chemical, geological, biological, and land-use characteristics similar to the site, as described in Guide E3164, Appendix X2. Extraction of representative background data from site data often involves utilizing probability plots to segregate site data into impacted versus unimpacted populations for each PCOC (see Appendix X3).

10. Data Visualization

10.1 Evaluation of a candidate background data set should begin by visualizing the data. There are a number of techniques described in this section that can be used, depending on the characteristics of the data set. These plots are exploratory in nature and not all plots shown are required when visualizing the data set. Different plots depicting the same data set are illustrated in the following subsections. Other tools (for example, geographic information system [GIS] post plots) can also be used for data visualization.

10.2 *Dot Plots.* Dot plots represent each concentration in a data set as an individual dot (see Fig. 2), with concentration values listed along the *x*-axis (**15**). Samples with similar concentrations appear as vertical stacks, and large data sets can be accommodated by using one dot to represent a predetermined number of samples. This plot allows all samples to be viewed, and no distributional assumptions are imposed on the data. Symmetry, bimodal or multi-modal groupings, and skewness can also be discerned in dot plots.

10.3 *Histograms.* Histograms depict data sets in bar form, with concentrations (grouped in "bins," or intervals) along the *x*-axis and the corresponding frequency (or percentages of frequency) for each concentration interval along the *y*-axis (see Fig. 3). The area of each bar reflects the proportion of that concentration interval within the data set. Histograms are commonly used in conjunction with goodness-of-fit tests to assess the shape of a data distribution, because the graphs can reveal such features as symmetry, skewness, and bimodality. However, the observed shape of a data set is affected by the bin size (for example, 10 mg/kg interval versus 20 mg/kg interval), which should be carefully selected. Multiple data sets can be depicted on the same histogram using unique colors or patterns.

10.4 *Box Plots.* Box plots, or box-and-whisker plots, are used to compare two or more groups of data (**2, 16**). A box plot (see Fig. 4) provides a summary view of an entire data set, including the range of concentrations, degree of symmetry, and skewness of the data. The box encloses the central 50 % of the data points ("interquartile range"), with the top of the box representing the 75th percentile and the bottom of the box representing the 25th percentile; the median is represented by a symbol within the box. In this example, the upper whisker extends to the maximum data point and the lower whisker extends to the minimum data point. A side-by side configuration of box plots permits visual comparison of multiple data sets to quickly discern whether they are similar or distinct.

10.4.1 Users can define the appearance of box plots. Default settings in statistical software programs typically identify predefined "outlier values" (for example, values outside 1.5 times the interquartile range) and "extreme values" (for example, values outside 3 times the interquartile range). These settings are arbitrary and can be avoided by simply extending the upper and lower whiskers to the maximum and minimum data points. See also Section 11 and 13.1.2 for discussions of statistical outliers and their appropriate treatment.

10.5 *Probability Plots.* A probability plot is often used to visualize distributions and determine whether the data are normally or lognormally distributed (**2**). Probability plots can indicate the presence of possible outlier values, and they can help determine whether a single normal (or lognormal) distribution exists, as opposed to multiple distributions (see Fig. 5). The plots are constructed by rank-ordering the data and plotting each data point as the standard normal probability value for the respective rank on the *y*-axis and the concentration on the *x*-axis. For example, the normal probability value z_j for the j^{th} value (rank) in a sample with N observations is computed as: $z_j = M^{-1}\ [(3*j-1)/(3*N+1)]$, where M^{-1} = the inverse normal cumulative distribution function. A logarithmic scale on the *x*-axis is used for lognormal distributions (see Fig. 5), and a normal scale is used on the *x*-axis for normal distributions. If the points fall roughly on a straight line, one can conclude that the underlying data distribution is approximately normal (or lognormal), with the slope proportional to the variance of the data. Many environmental data sets do not fit parametric models (see 14.1), such as the normal or lognormal distribution, so probability plots can have limited utility or may lead to erroneous conclusions for those data sets.

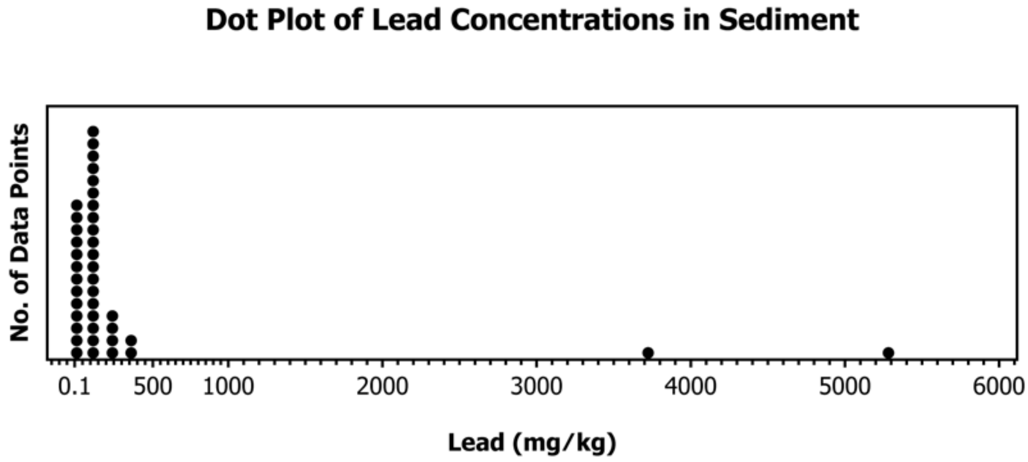

FIG. 2 Dot Plot of Lead Concentrations in a Set of Sediment Samples

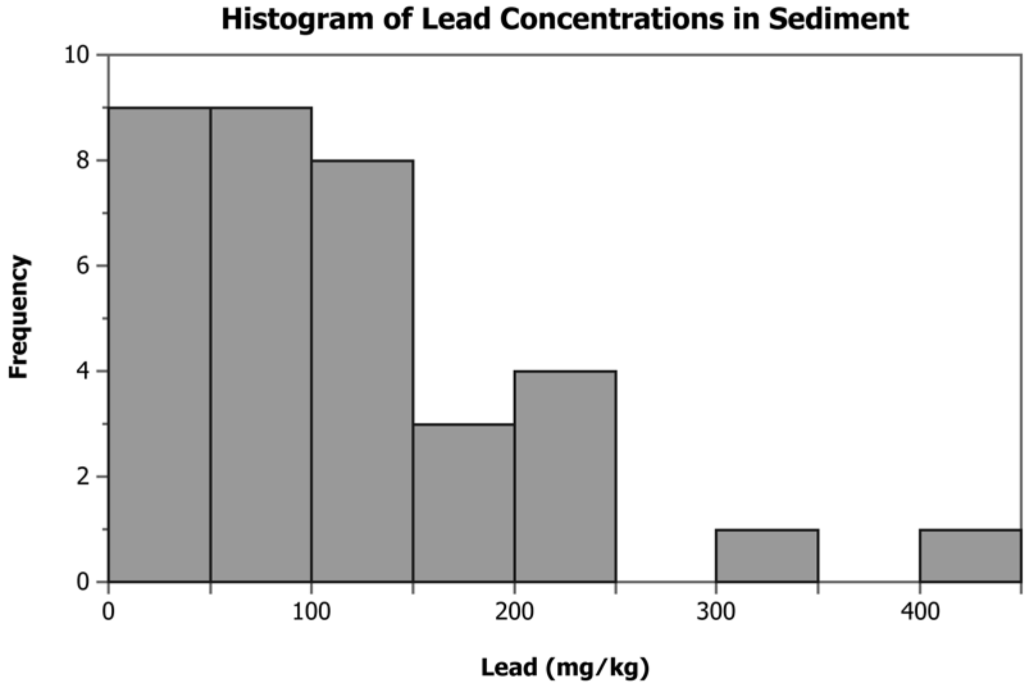

FIG. 3 Histogram of Lead Concentrations in a Set of Sediment Samples

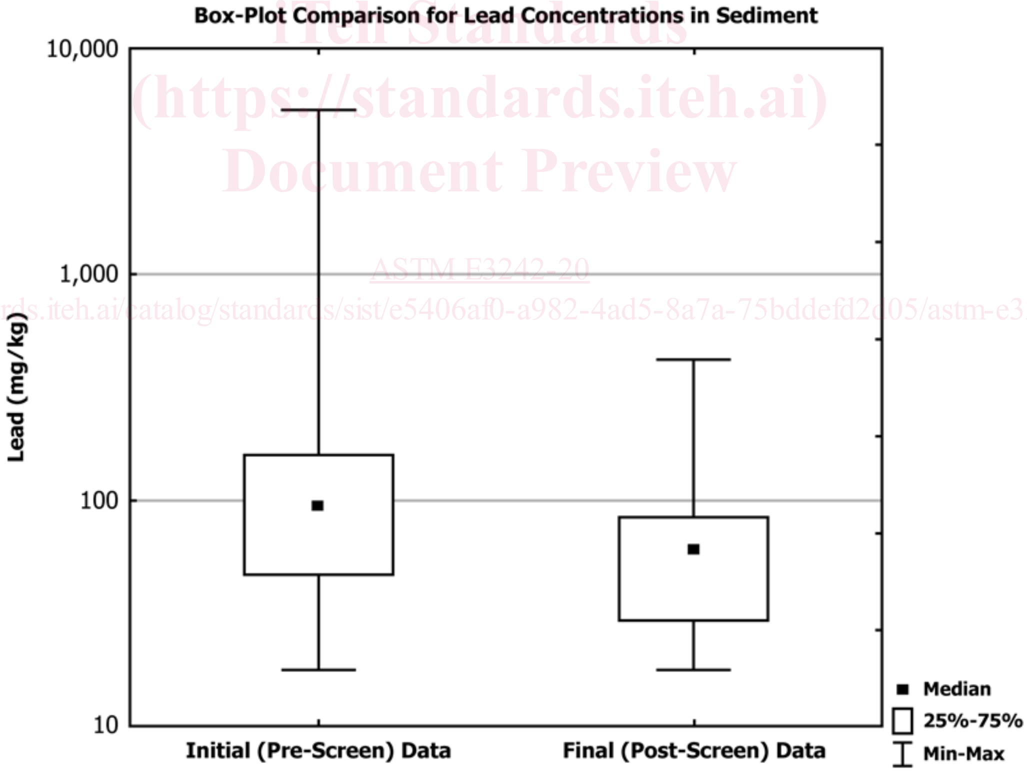

FIG. 4 Box Plots of Lead Concentrations in a Candidate Background Data Set (Left Side) and in the Final Background Data Set Following Screening Procedures (Right Side)

10.6 *Percentile Plots.* Percentile plots are similar to probability plots, but depict concentration versus percentile rather than concentration versus probability (see Fig. 6). The data are first rank-ordered and then concentrations are plotted on the *y*-axis with the corresponding percentiles plotted on the *x*-axis. Normally distributed data appear as a straight line if a linear concentration scale is used, and lognormally distributed data appear as a straight line if a logarithmic concentration scale is used; statistical outliers will appear above or below the linear trend. A break in slope may be observed if the distribution is

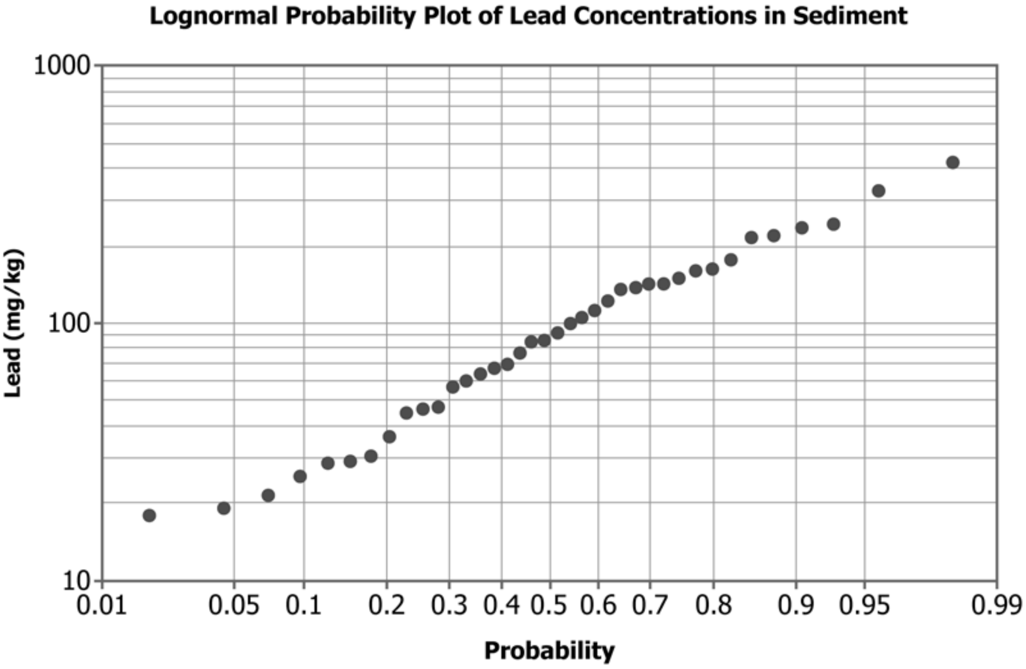

FIG. 5 Lognormal Probability Plot of Lead Concentrations in a Set of Sediment Samples

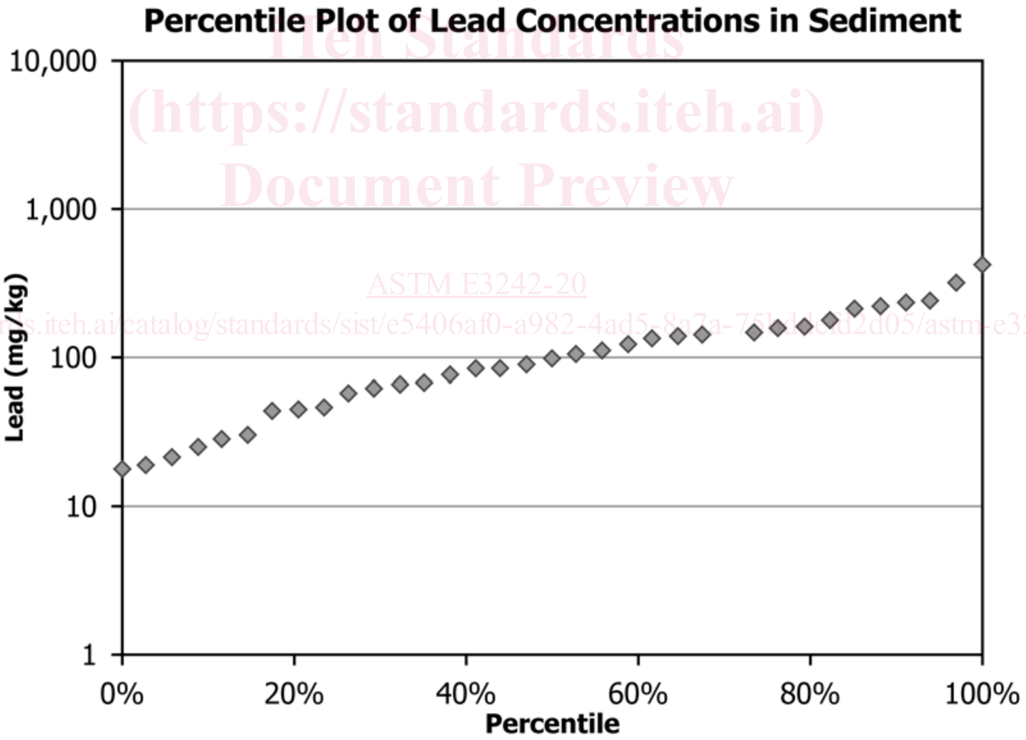

FIG. 6 Nonparametric Percentile Plot of Lead Concentrations in a Set of Sediment Samples

bimodal or if multiple samples have identical concentrations. As with probability plots, percentile plots permit a qualitative assessment of the shape of the data. A key advantage of percentile plots is that they are nonparametric, so they can be used to visualize any data set without making assumptions regarding the distributional shape of the data set.

10.7 *Scatter Plots.* In support of the geochemical evaluation of metals data, scatter plots are constructed to explore elemental associations and identify potentially contaminated samples (**17**). Trace element concentrations are plotted along the *y*-axis and the corresponding reference element concentrations (typically major elements such as iron and aluminum) are plotted along the *x*-axis (see Fig. 7). The reference element represents the mineral to which the trace element may be adsorbed, as discussed in 12.4. A common trend (not necessarily linear) is observed in the absence of contamination, due to similar trace-versus-reference element ratios. A sample with excess trace element from a contaminant source will exhibit an anomalously high trace-versus-reference element ratio relative to unimpacted samples and will lie above the trend.

10.8 *Ratio Plots.* Ratio plots are recommended to accompany each scatter plot **(18)**. Ratio plots depict trace element concentrations along the *y*-axis and the corresponding elemental ratios (that is, the trace element concentration divided by the reference element concentration for each sample) along the *x*-axis (see Fig. 8). Unimpacted samples exhibit consistent trace-versus-reference element ratios. A sample with excess trace element from a contaminant source will exhibit an anomalously high trace-versus-reference element ratio relative to unimpacted samples and will lie to the right of the unimpacted samples in the ratio plot.

11. Evaluation of Outliers

11.1 Representative background concentrations may contain outlying observations, or "outliers," that appear to deviate markedly from other members of the sample set in which they occur. There are well-established procedures to test for statistical outliers (refer to Appendix X4, Table X4.1). Each statistical test requires a pre-identified number of probable or perceived high and/or low outliers and an assumed distribution of the background population. Typical occurrences include a single outlier, or two or more outliers on the same or opposite sides of the data set.

11.2 Common statistical outlier tests, including those presented in Practice E178, typically assume the normality of the data set after the removal of outliers. For many environmental data sets, the normality assumption is incorrect, which can lead to erroneous outlier identifications. This problem is further exacerbated when the above statistical tests are applied repeatedly, through the iterative removal of perceived outliers. Under such procedures, shrinking standard deviations caused by continuous exclusion of perceived outliers produces an increasing likelihood of incorrect identification of additional outliers. The end result is the calculation of biased, unrepresentative background concentrations from an incorrectly truncated background data set. Therefore, graphical techniques (see Section 10) may be more appropriate for identifying outliers.

11.3 Practice E178 classifies the identified outliers into two broad groups:

11.3.1 "An outlying observation might be the result of gross deviation from prescribed experimental procedure or an error in calculating or recording the numerical value. When the experimenter is clearly aware that a deviation from prescribed experimental procedure has taken place, the resultant observation should be discarded, whether or not it agrees with the rest of the data and without recourse to statistical tests for outliers. If a reliable correction procedure is available, the observation may sometimes be corrected and retained."

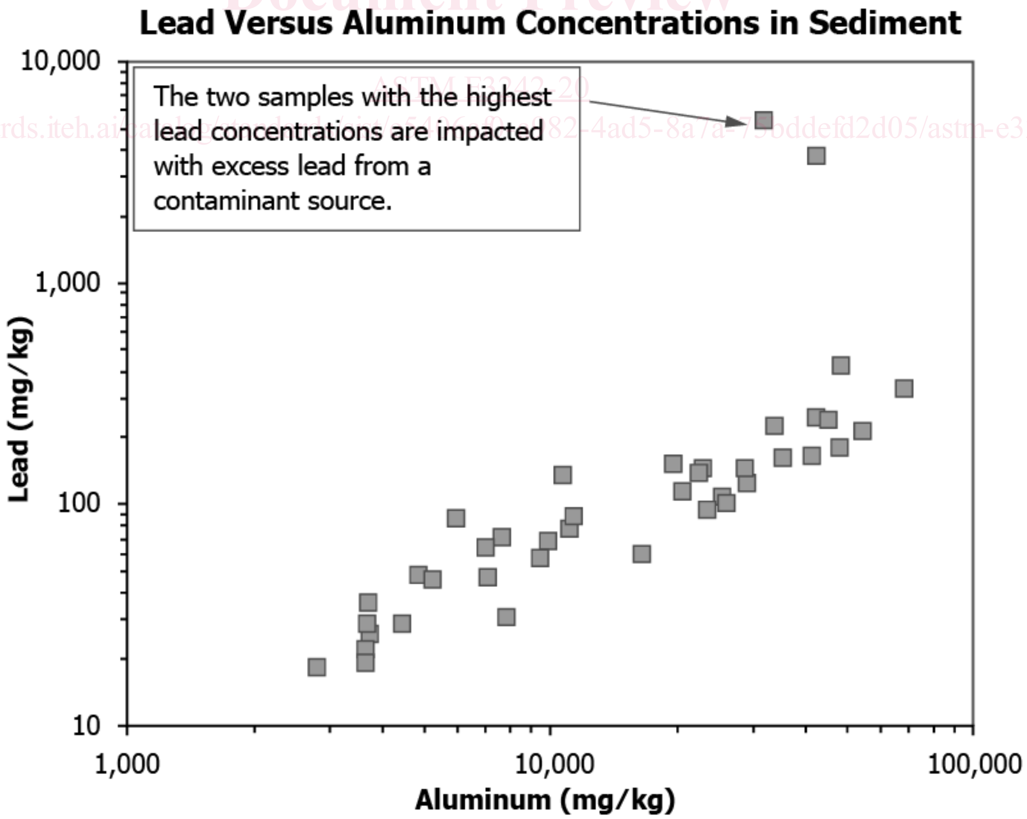

FIG. 7 Scatter Plot of Lead Concentrations Versus Aluminum Concentrations in a Set of Sediment Samples

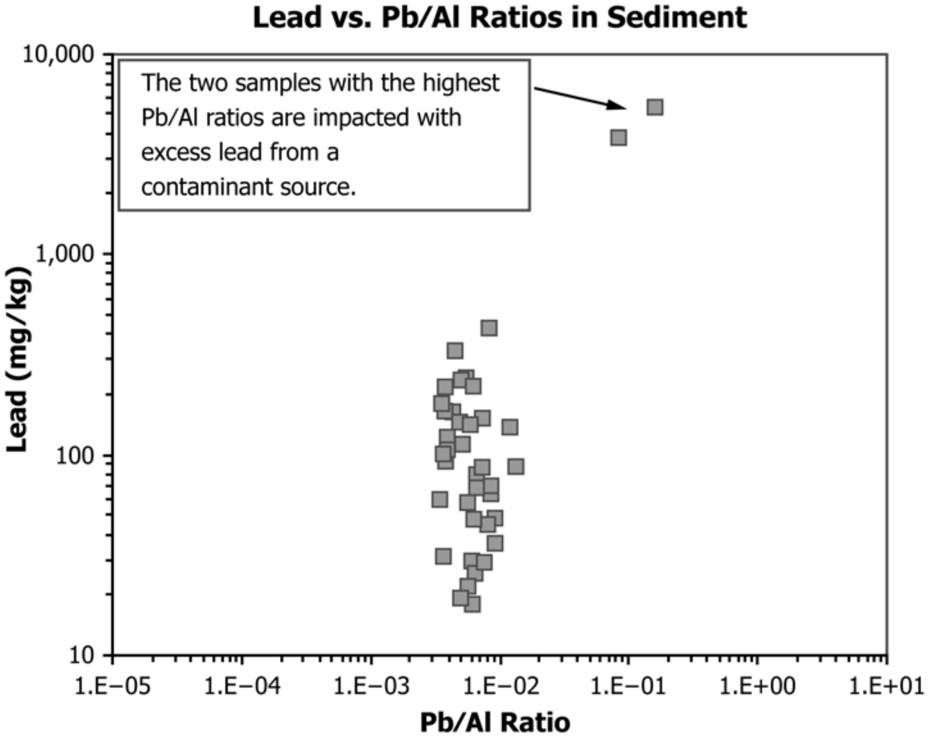

FIG. 8 Ratio Plot Depicting Lead Concentrations Versus Lead/Aluminum Ratios in a Set of Sediment Samples

11.3.2 "An outlying observation might be merely an extreme manifestation of the random variability inherent in the data. If this is true, the value should be retained and processed in the same manner as the other observations in the sample. Transformation of data or using methods of data analysis designed for a non-normal distribution might be appropriate."

11.4 Section 4.4. of (2) refers to the above two types of outlying observations as "true" outliers and "false" outliers, respectively. The USEPA guidance (2) states that "failure to remove true outliers or the removal of false outliers both lead to a distortion of estimates of population parameters." In practice, only outliers that are demonstrably erroneous or belong to populations not representative of background conditions should be excluded. All other identified outliers should be retained and processed in the same manner as the other observations in the sample. A comprehensive review of outlier removal issues is presented in (19).

12. Chemical and Geochemical Evaluations

12.1 This section focuses on metals for several reasons. Of note are the differences between metals and organics, which require distinct types of evaluations. The biggest difference is that all elements are naturally occurring (although some organics like PAHs can also occur naturally). Their natural occurrence makes it necessary at some sites to distinguish between naturally occurring concentrations versus contamination. An additional difference is that the concentrations of metals are usually controlled by sorption reactions on specific mineral surfaces, which enables evaluations of the ratios of the contaminants versus the concentrations of major elements in the host minerals. These ratios can be used to identify the presence of contamination.

12.2 Many scientific papers thoroughly address the numerous environmental forensic techniques that can be employed for source attribution of organic compounds (for example, (5, 6, 9, 11, 20, 21, 22, 23, 24, 25, 26)) and they are often used during background sediment studies. However, regulatory guidance documents do not provide an analogous methodology for the evaluation of metals concentrations, which can be naturally elevated in sediment and—on the basis of absolute concentrations alone—can appear to reflect contaminant input even in the absence of anthropogenic sources. Instead, regulatory guidance documents tend to focus solely on statistical methods when characterizing background data sets for metals. Based on the above, the focus of this section is metals.

12.3 Multiple processes control the concentrations of elements in sediment, and it is important to consider these processes when identifying a representative background data set, evaluating statistical outliers, and comparing analyses of site versus background samples. These processes include adsorption-desorption reactions (generally the most important among the various processes), dissolution-precipitation reactions, oxidation-reduction (redox) effects, and pH effects. At any given site, an element's concentrations may be controlled by one or more of these processes, which can be highly localized phenomena. For example, a trace element such as nickel may adsorb on the surfaces of iron oxide minerals or