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Standard Guide for Generation of Environmental Data Related to Waste Management Activities: Selection and Optimization of Sampling Design[1]

This standard is issued under the fixed designation D 6311; 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 document provides practical guidance on the selection and optimization of sample designs in waste management sampling activities, within the context of the requirements established by the data quality objectives or other planning process.

1.2 This document (*1*) provides guidance for selection of sampling designs; (*2*) outlines techniques to optimize candidate designs; and (*3*) describes the variables that need to be balanced in choosing the final optimized design.

1.3 The contents of this guide are arranged by section as follows:

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 and health practices and determine the applicability of regulatory limitations prior to use.*

2. Referenced Documents

2.1 *ASTM Standards:*

D 4687 Guide for General Planning of Waste Sampling[2]

D 5283 Practice for Generation of Environmental Data Related to Waste Management Activities: Quality Assurance and Quality Control Planning and Implementation[2]

D 5792 Practice for Generation of Environmental Data Related to Waste Management Activities: Development of Data Quality Objectives[2]

D 5956 Guide for Sampling Strategies for Heterogeneous Wastes[2]

D 6044 Guide for Representative Sampling for Management of Waste and Contaminated Media[2]

D 6051 Guide for Composite Sampling and Field Subsampling for Environmental Waste Management Activities[2]

D 6232 Guide for Selection of Sampling Equipment for Waste and Contaminated Media Data Collection Activities[2]

D 6233 Guide for Data Assessment for Environmental Waste Management Activities[2]

D 6250 Practice for Derivation of Decision Point and Condifence Limit for Statistical Testing of Mean Concentration in Waste Management Decisions[2]

D 6323 Guide for Laboratory Subsampling of Media Related to Waste Management Activities[2]

E 135 Terminology Relating to Analytical Chemistry for

[1] This guide is under the jurisdiction of ASTM Committee D34 on Waste Management and is the direct responsibility of Subcommittee D34.01.01 on Planning for Sampling.

Current edition approved Sept. 10, 1998. Published November 1998.

[2] *Annual Book of ASTM Standards*, Vol 11.04.

Metals, Ores and Related Materials[3]

E 943 Terminology Relating to Biological Effects and Environmental Fate[4]

2.2 *USEPA Documents:*

USEPA, Guidance for the Data Quality Objectives Process, EPA QA/G-4, Quality Assurance Management Staff, Washington, DC, March 1995[5]

USEPA, Data Quality Objectives Process for Superfund - Workbook, EPA 540/R-93/078 (OSWER 9355.9-01A), Office of Emergency and Remedial Response, Washington, D.C., September, 1993[5]

USEPA, Environmental Investigations Branch Standard Operating Procedures and Quality Assurance Manual (EISOPQAM), Region 4 - Science and Ecosystem Support Division, Athens, GA, May 1996[5]

2.3 There are numerous useful references available from ASTM, USEPA, and private sector publishers. Appendix X1 contains a list, which is by no means comprehensive, of additional commonly used references.

3. Terminology

3.1 *accuracy*, *n*—closeness of a measured value to the true or an accepted reference or standard value. **(E 135)**

3.2 *attribute*, *n*—a quality of samples or a population. **(D 5956)**

3.3 *characteristic*, *n*—a property of items in a sample or population that can be measured, counted, or otherwise observed. **(D 5956)**

3.3.1 *Discussion*—A characteristic of interest may be the cadmium concentration or ignitability of a population.

3.4 *composite sample*, *n*—a combination of two or more samples.

3.5 *confidence interval*, *n*—a numerical range used to bound the value of a population parameter with a specified degree of confidence (that the interval would include the true parameter value).

3.5.1 *Discussion*—When providing a confidence interval, the number of observations on which the interval is based should be identified.

3.6 *confidence level*, *n*—the probability, usually expressed as a percent, that a confidence interval will contain the parameter of interest.

3.7 *data quality objectives (DQO)*, *n*—qualitative and quantitative statements derived from the DQO process describing the decision rules and the uncertainties of the decision(s) within the context of the problem(s). **(D 5956)**

3.8 *data quality objective process*, *n*—a quality management tool based on the scientific method and developed by the U.S. Environmental Protection Agency to facilitate the planning of environmental data collection activities. **(D 5956)**

3.8.1 *Discussion*—The DQO process enables planners to focus their planning efforts by specifying the use of the data (the decision), the decision criteria (action level) and the decision maker's acceptable decision error rates. The products of the DQO Process are the DQOs.

3.9 *decision rule*, *n*—a set of directions in the form of conditional statements that specifies: (*1*) how the sample data will be compared to the decision point or action level, (*2*) which decision will be made as a result of that comparison, and (*3*) what subsequent action will be taken based on the decisions.

3.10 *false negative error*, *n*—an error which occurs when (environmental) data misleads the decision maker(s) into not taking action when action should be taken.

3.11 *false positive error*, *n*—an error which occurs when environmental data misleads the decision maker(s) into taking action when action should not be taken.

3.12 *heterogeneity*, *n*—the condition of the population under which items of the population are not identical with respect to the characteristic of interest. **(D 5956)**

3.13 *homogeneity*, *n*—the condition of the population under which all items of the population are identical with respect to the characteristic of interest. **(D 5956)**

3.14 *representative sample*, *n*—a sample collected such that it reflects one or more characteristics of interest (as defined by the project objectives) of a population from which it was collected. **(D 5956)**

3.15 *risk*, *n*—the probability or likelihood that an adverse effect will occur. **(E 943)**

3.16 *sample*, *n*—a portion of material which is collected for testing or for record purposes. **(D 5956)**

3.16.1 *Discussion*—Sample is a term with numerous meanings. The project team member collecting physical samples (for example, from a landfill, drum or waste pipe) or analyzing samples considers a sample to be that unit of the population collected and placed in a container. In statistics, a sample is considered to be a subset of the population and this subset may consist of one or more physical samples. To minimize confusion, the term "physical sample" is a reference to the sample held in a sample container or that portion of the population which is subjected to measurement.

3.17 *sampling design*, *n*—(*1*) the sampling schemes specifying the point(s) for sample collection; (*2*) the sampling schemes and associated components for implementation of a sampling event.

3.17.1 *Discussion*—Both of the above definitions are commonly used within the environmental community. Therefore, both are used within this document.

4. Significance and Use

4.1 The intended use of this guide is to provide practical assistance in the development of an optimized sampling design. This standard describes or discusses:

4.1.1 Sampling design selection criteria,

4.1.2 Factors impacting the choice of a sampling design,

4.1.3 Selection of a sampling design,

4.1.4 Techniques for optimizing candidate designs, and

4.1.5 The criteria for evaluating an optimized sampling design.

[3] *Annual Book of ASTM Standards*, Vol 03.05.

[4] *Annual Book of ASTM Standards*, Vol 11.05.

[5] Available from the Superintendent of Documents, U.S. Government Printing Office, Washington, DC 20402.

4.2 Within a formal USEPA data generation activity, the planning process or Data Quality Objectives (DQO) development is the first step. The second and third are the implementation of the sampling and analysis design and the data quality assessment. Within the DQO planning process, the selection and optimization of the sampling design is the last step, and therefore, the culmination of the DQO process. The preceding steps in the DQO planning process address:

4.2.1 The problem that needs to be addressed,

4.2.2 The possible decisions,

4.2.3 The data input and associated activities,

4.2.4 The boundaries of the study,

4.2.5 The development of decision rules, and

4.2.6 The specified the limits on decision error.

4.3 This guide is not intended to address the aspects of the planning process for development of the project objectives. However, the project objectives must be outlined and communicated to the design team, prior to the selection and optimization of the sample design.

4.4 This guide references statistical aspects of the planning and implementation process and includes an appendix for the statistical calculation of the optimum number of samples for a given sampling design.

4.5 This guide is intended for those who are responsible for making decisions about environmental waste management activities.

5. Summary of Guide

5.1 The selection and optimization process is an iterative process of selecting and then evaluating the selected design alternatives and determining the most resource-effective design which satisfies the project objectives or DQOs. Fig. 1 illustrates this approach.

5.2 An appropriate sampling design may be implemented without a formal optimization, however, the following steps are recommended. Each evaluation step typically results in fewer design alternatives.

5.2.1 Evaluation of the designs against the project's practical considerations (for example, time, personnel, and material resources),

5.2.2 Calculation of the design cost and statistical uncertainty, and

5.2.3 Choice of the sample design decision by the decision makers.

5.3 The process steps for the evaluation can be followed in any order. And for a small project, the entire selection and optimization process may be conducted at the same time. If ultimately, a design meeting the project constraints, for example, schedule and budget, cannot be identified among the candidate sampling designs, it may be necessary to modify the closest candidate design or reevaluate and revise the project objectives.

6. Factors Affecting Sampling Design Selection

6.1 *Sampling Design Performance Characteristics*:

6.1.1 The sampling design provides the structure and detail for the sampling activity and should be chosen in light of the project objectives. Prior to this point, the planning process should have addressed and defined the project needs for each of the sampling design characteristics, including the characteristics of interest, population boundaries, decision rule, acceptable decision errors and budgets. In considering all aspects of the project, the selected design should accommodate the spatial and temporal distribution of contaminants at the site, be practical, cost effective and generate data that allow the project objectives to be met.

6.1.2 Whenever possible, technical guidelines for measurement of the sources of variability and levels of uncertainty should be established prior to developing sampling design alternatives, to ensure that it is possible to establish that the program objectives are met.

6.1.3 Annex A1 presents an overview of some of the more commonly used sampling designs and design tools and summarizes their advantages and disadvantages. Because numerous sampling strategies exist, this is limited to the more common. If the more common sampling strategies are not cost-effective or applicable to the population of interest, a statistician should be consulted to identify other strategies which may be more appropriate.

6.2 *Regulatory Considerations*—The selection of sampling design, the sampling techniques and analytical methods may be dictated by current regulation, permits or consent agreements, applicable to the site. These should be reviewed to determine their impact on the selection process.

6.3 *Project Objectives*—Project objectives are usually determined by the decision makers (for example, regulatory body, consent agreement group, company management) during the initial investigation and planning or DQO process. The decision makers should have identified the population boundaries, characteristics of interest, acceptability of an average analytical value, the need to locate areas of contamination or "hot spots," the statistical needs (for example, acceptable decision errors, levels of uncertainty), and the quality control acceptance criteria, as well as any other pertinent information.

6.4 *Knowledge of the Site*—The site knowledge (for example, geography/topography, utilities, past site use) used to determine project objectives, will also provide for a more resource efficient sampling design, for example, divide a site into separate design areas for sampling or exclude an area from sampling.

6.5 *Physical Sample Issues*—The physical material to be sampled and its location on or within the site will usually impact the sampling design and limit the choices of equipment and methods.

6.5.1 *Number of Samples*:

6.5.1.1 The project objectives should specify the confidence levels for decision making. Using this level of decision error, the proximity to a threshold or action limit and the anticipated population variance, the number of samples can be calculated. The statistical parameter of interest, for example, mean or 95 percentile, and type of frequency of distribution, for example, normal or log normal, will determine which equation is used to calculate the appropriate number of samples. Equation X3.5 from Appendix X3, can be used to calculate the number of samples when the objective is to measure the mean for a population that has a normal distribution for the characteristic of interest.

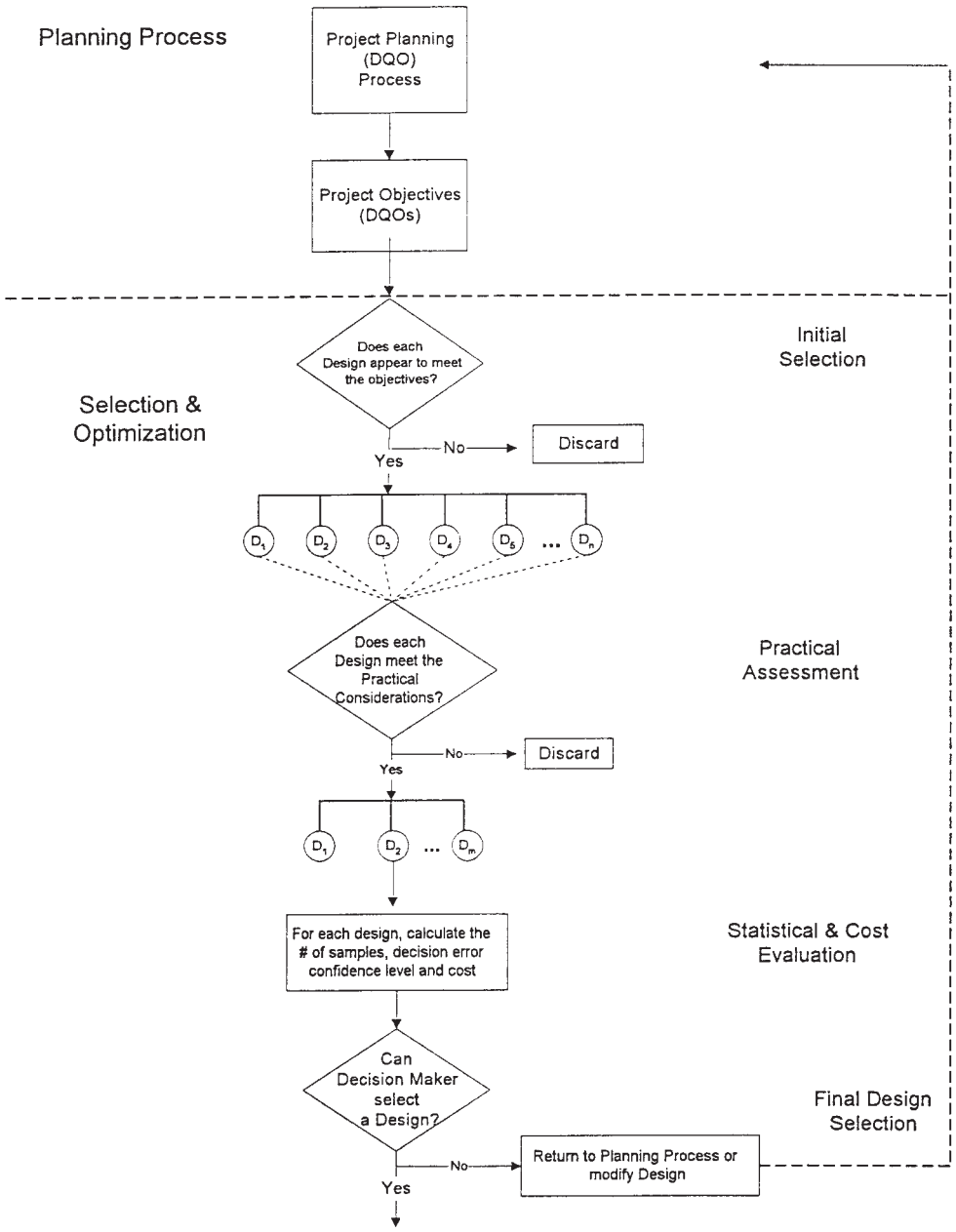


FIG. 1 Implement Sampling Design

6.5.1.2 Appendix X3 contains statistical approaches to calculating the number of samples needed for estimating the mean concentration, for simple random, statistical random, multistage sampling and search sampling (where the objective is to detect hot spots).

6.5.2 *Sample Mass or Volume*:

6.5.2.1 The sample mass or volume is determined by the size of the items that constitute the population, the heterogeneity of the population, the characteristics of available sampling equipment (for example, dimensions) and the mass or volume needed for analysis.

6.5.2.2 It is important that the sample mass be large enough to accommodate all item sizes or parts of all items. If items such as fine granular sand or large discarded automobile parts constitute the population, the sample may need to include those items or wipes of those items.

6.5.3 *Sample Access and Logistics*—Site access and logistics such as the following, can alter the sampling design:

6.5.3.1 Whether equipment can maneuver on site to obtain the desired samples,

6.5.3.2 Availability of power and water,

6.5.3.3 Presence of buried, suspended or surficial utilities, for example, power lines, water lines, etc.,

6.5.3.4 Terrain including slope, stability of site (subsidence considerations), presence of brush or trees, and soil condition (hard pack versus mud), and

6.5.3.5 Noise of equipment which could constitute a nuisance.

6.5.3.6 For further information, see Guide D 6232 and Guide D 5956.

6.5.4 *Sample Matrix*:

6.5.4.1 The physical properties of the matrix to be sampled will determine the suitability of some sampling devices. Some devices work best with cohesive material, such as moist soils, while other work best with dry materials. Equipment used to dig, core and sample abrasive materials needs to be strong enough to maintain its integrity during sampling. The sampling program should not be compromised by incompatibilities between the sampling device and the waste.

6.5.4.2 Heterogeneity will impact both the sampling design and the physical means of collecting the samples. Non-uniform distribution of the contaminant(s) of interest and/or varying particle size of the material, for example, soil, concrete, building material, vegetation, will require different sampling equipment and sampling strategies. For further information, see Guide D 6232 and Guide D 5956.

6.6 *Communication with the Laboratory*—Advanced planning with the laboratory should address the sampling schedule, sample preparation techniques, any subsampling instructions, analytical procedures, analytes of interest, matrices to be analyzed, data report format, data to be reported, and any specific requirements for accuracy, precision, quality control, calibration and needed turn around time.

6.7 *Analytical Turn Around Time*—Turn around time is usually the time from sample receipt in the laboratory to analytical data delivery. This usually depends on the analytical considerations and the laboratory capabilities.

6.8 *Analytical Method Constraints*—The analytical methods need to be chosen prior to or in conjunction with the optimization of the sampling design. The selection of appropriate methods needs to take into account at least the following areas.

6.8.1 *Analytical Method Sensitivity*—The analytical method sensitivity, usually expressed as the method detection limit or detection limit, may dictate the mass or volume of sample needed, the selection of the analytical methods, and the accuracy and precision of the data. Analytical method sensitivity is influenced by a number of factors, including sample preparation, sample volume, percent moisture, dilutions, and analytical method used.

6.8.1.1 *Analytical Aliquot Mass or Volume*—In general, for a given method, the larger the analytical aliquot (up to the maximum accommodated by the analytical method), the lower the detection limit and the more representative the data. However, typical aliquots used by most methods range from a few milliliters to 1 L or 100 g. The laboratory instrumentation may not be physically capable of managing a much larger aliquot.

6.8.1.2 *Dilutions*—Any analytical dilution will decrease sensitivity and increase the detection limit, as a multiplier of the dilution factor. When the sample has parameters in high concentrations, the lab may dilute the sample to allow the parameter to fall within the analytical instruments' calibration range.

*(1)*Samples containing parameters of varied concentrations may need to be prepared and analyzed at different dilutions. The manner of reporting these multiple analyses need to be agreed upon with the laboratory prior to analysis.

6.8.1.3 *Action Levels*—Detection levels need to be lower than the decision points or regulatory levels. If the detection limit is at the action or regulatory level, the increased levels of imprecision will increase the uncertainty in the decision. Low detection limit requirements may require special method development. The validation and ruggedization of new methods can be costly and impact schedules.

6.8.2 *Moisture Content of Samples*—Reporting analytical results on a dry weight basis may increase the sample mass requirements. Dry weight reporting may be accomplished in one of two ways.

6.8.2.1 Dry the sample aliquot prior to analysis on the same sample aliquot. This approach usually yields the lower detection limit. However, drying may change the sample. For example, it may affect the results of an analytical extraction, such as oxidizing a constituent, for example, hexavalent chromium.

6.8.2.2 Employ two sample aliquots. One aliquot is used to determine the moisture content, which is then used to calculate a dry weight analytical result, based on an analysis of the second aliquot. This second approach can result is raised detection limits, but it is required for the analysis of volatile analytes, which would be lost during drying.

6.8.3 *Holding Times*—The holding time is usually the time from sample collection to sample extraction or analysis. Most regulatory agencies will not accept or will limit the use of data from a sample analyzed outside the specified holding time. Holding times differ depending on the media, analyte, and regulation.

6.8.3.1 Analyses such as pH, hexavalent chromium, semivolatile and volatile organics have short holding times and may necessitate special planning. Samples with very short holding times will need to be shipped as soon as possible to allow sufficient processing time or will need on-site analysis.

6.8.4 *Screening Measurements*:

6.8.4.1 *Screening*—Screening methods can implemented in the field or the laboratory and can provide either qualitative or semi-quantitative analyses. Screening methods are faster and generally less costly than traditional laboratory methods, but may be less sensitive and employ less quality control than traditional methods. However, they allow field personnel to define problematic areas quickly and to guide the sampling and verification analyses, using traditional methods, for final compliance determination.

6.8.4.2 *Field and In-Situ Analyses*—When hold or turn around times cannot be met by traditional laboratory analyses or to save time, reduce cost, or increase the number of samples, analytical testing may be performed at the sampling site. Field analytical methods include chemical specific kits and portable instrumentation for various organic and inorganic compounds. Care should be taken that the needed detection limits, regulatory requirements and quality control are achievable and that accuracy and precision criteria, trained staff, and data management practices are in place to produce data to meet the planning objectives or DQOs.

6.9 *Health and Safety*—Personnel safety must be considered. Of particular concern are any potential exposure of field personnel to hazardous materials and any possibility for explosion or fire which might be triggered by sampling equipment. Additionally, intrusive sampling, such as drilling, can result in the release of hazardous materials to the environment and potentially impact off-site personnel.

6.10 *Budget/Cost Considerations*—Budgets are almost always a significant factor. The challenge is to design a cost-effective sampling plan, while still achieving the specified project objectives. The sample design cost estimate comparisons need to include:

6.10.1 Personnel costs including travel and per diem,
6.10.2 Sampling equipment, including purchases/rentals,
6.10.3 Mobilization and demobilization costs,
6.10.4 Decontamination of equipment,
6.10.5 Waste collection and disposal,
6.10.6 Sample analyses and/or field screening,
6.10.7 QA or QC samples, or both,
6.10.8 Consumables, and
6.10.9 Health and safety.

6.11 *Representativeness*—Representativeness is the degree to which samples collected reflect the characteristics of the population. The sampling design must be chosen such that bias is minimized and the other project objectives achieved. For further guidance, see Guide D 6044.

7. Initial Design Selection

7.1 Sampling design options need to be selected consistent with the project objectives. Prior to selecting designs, the parameter(s) of interest (target compounds), population boundaries, decision rule, the spatial and temporal distribution of contaminants at the site (if known), the acceptable decision errors and budgets should have been considered in the planning process. In addition the final design should be practical and cost-effective. See Annex A1 for a listing of commonly used sampling designs.

7.2 *Meeting Project Objectives*—Prior to the selection of the initial set of sampling designs, those responsible for the project planning or DQO process need to establish and communicate the project objectives. Fig. 2 provides a guide to some common sampling designs as they could potentially satisfy some basic project objectives. Fig. 3 gives a guide to some of the attributes of the same designs.

7.2.1 *Estimating Population Parameters*—Waste classification, evaluation of waste treatability or determining compatibility of wastes are types of projects where information of the population parameters, such as the mean and variance, may be required. Estimation of these parameters generally relies on a statistical sampling design and classical inferential statistics.

7.2.2 *Monitoring for Routine Purposes*—Monitoring, such as ground water or monitoring changes in waste streams over time may be useful in determining for example whether a characteristic of a waste stream has exceeded a prespecified quality control or permit limit.

7.2.3 *Describing Spatial or Temporal Distribution, or Both*—Information for corrective action purposes may be used to define spatially or temporally those portions of a waste stream that are to be managed in different ways (for example, disposal versus treatment, etc.) Information may also be used for locating additional sampling units for increased precision in defining boundaries separating wastes to be manage differently.

7.2.4 *Non-Compliance Monitoring*—Identifying hot spots is a common non-compliance monitoring objective. Search sampling is used to locate or detect constituents of interest, objects," hot spots" in the area to be sampled. Authoritative sampling based on site knowledge is frequently used to identify the possibility of the "worst case" scenario non-compliance.

7.3 *Sampling Designs for Complex Sites*—Many sites for environmental sampling are complex and require the selection of multiple sampling designs to address the various suspected problems. For these sites, optimization of several sample designs is needed. Once the specific areas are defined, the process is similar to any other optimization. The following is an example.

7.3.1 *Example*—Fig. 4 illustrates a complex site, one where a multi-design program is appropriate. It represents a source of

	Sampling Designs							
	Authoritative		Statistical				Systematic	
Objectives \ Sampling Designs	Judgmental	Biased	Simple Random	Stratified	Search	Unequal Probability	Line	Grid
Estimate population parameters			✓	✓				✓
Routine Monitoring	✓		✓	✓			✓	
Describe spatial and/or temporal distribution				✓	✓	✓	✓	✓
Non-Compliance Monitoring	✓	✓			✓			

FIG. 2 Project Objectives and Sampling Designs Guidance

Sampling Designs / Attributes	Designs: Authoritative		Statistical				Systematic	
	Judgmental	Biased	Simple Random	Stratified Random	Search	Unequal Probability	Line	Grid
Some Knowledge of Contaminant Distribution	✓	✓		✓		✓		
Usually is less Costly	✓	✓						
Simple to Implement	✓	✓	✓				✓	✓
Estimates Average Conditions			✓	✓		✓	✓	✓
Estimates Variability			✓	✓				✓
Minimizes Personal Bias			✓	✓			✓	✓
Effectively Accommodates and Identifies Strata				✓			✓	✓
Identifies or Locates Hot Spots		✓			✓			✓
Considers Trends or Cycles in Contaminant Distribution						✓		✓
Identifies Trends and Cycles in Contaminant Distribution							✓	✓

FIG. 3 Relationships Between Sampling Designs and Some Attributes Guidance

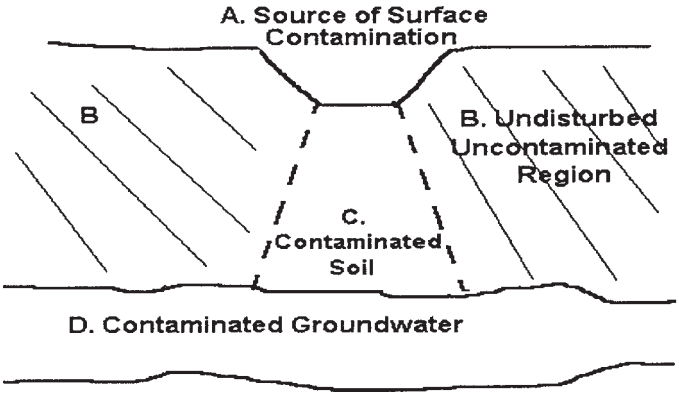


FIG. 4 Complex Site

potential contamination such as a waste lagoon that is leaking contaminated liquids to the subsurface and the ground water. To determine the extent of the problem, it is necessary to collect samples from separate areas of the site and answer the following:

7.3.1.1 What are the potential contaminants present in the lagoon?

7.3.1.2 What are the background levels of contaminants?

7.3.1.3 What are the levels of the potential contaminants in the soil immediately adjacent to and beneath the lagoon?

7.3.1.4 Has the contamination reached the ground water and to what extent?

7.3.2 Assuming the planning team is familiar with the process waste and the spatial heterogeneity of the lagoon, the first question can be answered by an authoritative sampling. The second question can be answered by a systematic sampling of the areas adjacent to the site. The answer to the third question can be found by a systematic sampling design around and beneath the lagoon. The fourth question can be answered by a systematic sampling of the ground water along a line from the point of origin (the lagoon) in the direction of ground water flow.

7.3.3 The final integrated plan for the entire site should consider all the information needs integrate multiple sampling designs (per area) and stage the field sampling to collect samples in such a manner that it will satisfy more than one area or question. For example, samples from the lagoon can be scheduled first and the results used to determine the analyte list for the soils and ground water. The soil borings used to determine the contamination around and beneath the lagoon and the ground water samples from the ground water beneath the site will provide information about the extent of any plume. This type of integrated planning occurs after the selection of the designs to answer the individual questions. Many times, considerable cost savings can be realized by this type of selection and optimization.

	Area of Site and Description	Candidate Design
A.	Lagoon (source of the contamination)	Authoritative Sampling
B.	Undisturbed soil area (presumed uncontaminated)	Systematic Sampling
C.	Soil directly under the spill (known to be contaminated, need to map extent of contamination)	Systematic Sampling
D.	Ground water (need to know the extent of contamination of ground water plume)	Grid Sampling

7.4 *Statistical versus Non-statistical Designs*:

7.4.1 *Non-Statistical Designs*—Sampling designs can be classified as statistical or non-statistical sampling designs. Non-statistical sampling designs are sometimes referred to as non-probability or authoritative (biased or judgmental) sampling. These strategies rely upon a person's judgment or a pre-arranged decision-rule to decide which portions of a population will be sampled. Non-statistical sampling designs can be the optimum strategy for certain populations or times in a sampling program. Non-statistical sampling may be appropriate under circumstances such as the following: (*1*) pilot studies (preliminary information is needed to facilitate planning); (*2*) spills: a spill of an unknown chemical has been encountered; (*3*) limited access to portions of the population; (*4*) field screening to select a limited number of samples for laboratory analysis; (*5*) historical site knowledge is available; and (*6*) non-compliance determinations.

7.4.1.1 While non-statistical sampling can generate useful data, because of its subjective nature, the logic used to choose the sampling location must be explained and defensible.

7.4.1.2 It is very important not to confuse non-statistical sampling with the use of historical information during sampling design. For example, if one area of a site is known to be heavily contaminated while another area is believed not to be contaminated, this information can be used to defensibly divide the site into strata or de-select an area from sampling. Use of historical information in conjunction with statistical sampling strategies should generate unbiased, representative and defensible data.

7.4.2 *Statistical Designs*—Statistical sampling designs are also referred to as probability, non-biased or non-judgmental designs and rely upon a random selection of sampling locations to minimize any bias in the sample selection process. Statistical sampling strategies allow for large populations to be characterized with a measured degree of confidence. In addition to considering all the other information, the following may apply:

7.4.2.1 Usually, the greater the number of samples, the narrower or tighter the confidence interval for the parameter of interest.

7.4.2.2 Composite samples are useful for locating the hot spot areas, although they may not identify a specific point source contaminant location.

7.4.2.3 For containerized waste, the sampling error for both the within (an individual) container and between multiple containers need to be considered.

7.4.2.4 Because sampling errors are usually larger and may be more difficult to quantify than analytical errors, field QC samples need to be included to help determine the potential errors.

7.4.2.5 Systematic grid sampling is preferred when spatial structure (correlation) is suspected or known. A random factor may be introduced by a random choice of origin. Systematic grid sampling usually provides a more accurate estimate of the mean.

8. Optimization Criteria

8.1 Optimization involves choosing between the initially selected sample designs which may or may not meet the project objectives. The optimum sample design will minimize project variables such as cost, time and risk, the objective being to achieve a balance between the costs of acquiring environmental data and the costs or consequences of incorrect waste management decisions.

8.2 In general the criteria for an optimized sampling design are that the design:

8.2.1 Be resource and cost effective,

8.2.2 Provide data of known quality,

8.2.3 Meet or not to exceed the acceptable level of decision errors,

8.2.4 Be practical or at least possible to implement, appropriately,

8.2.5 Comply with regulatory requirements,

8.2.6 Be implementable within the project schedule,

8.2.7 Have high reliability, and

8.2.8 Meet any other project specific objectives.

8.3 In the optimization process the above criteria will be used to choose the optimum design from the candidate sampling designs.

9. Optimization Process

9.1 The optimization process is an iterative process of evaluating the initially selected design alternatives and determining the most resource-effective design which satisfies the project objectives or DQOs. An appropriate sampling design may be implemented without a formal optimization, however, the following steps are recommended: (*1*) evaluation of the designs against the project's practical considerations (for example, time, personnel, and material resources); (*2*) calculation of the design cost and statistical uncertainty; and (*3*) choice of the sample design decision by the decision makers. Fig. 1 and Section 5, illustrate this approach.

9.1.1 The process steps for the evaluation can be followed in any order. For a small project, the entire selection and optimization process may be conducted simultaneously. Typically as the evaluation continues each evaluation step will result in fewer design alternatives. If, ultimately, a design meeting the project constraints, for example, schedule and budget, cannot be identified among the candidate sampling designs, it may be necessary to modify the closest candidate design or return to the planning stage and reevaluate and revise the project objectives.

9.2 *Practical Evaluation of Design Alternatives*—Each design candidate should be evaluated with respect to the project's practical considerations. These aspects should have been taken into account initially and some may overlap. However, the purpose here is to go into more depth and then to compare the design candidates. After reviewing, eliminate any designs which do not meet the site's practical needs.

9.2.1 *Define the Population or Area(s) to be Sampled*:

9.2.1.1 Review the site history and assumptions that were used to define the population boundaries. This information may allow for stratification of the site, identification of specific areas of interest and an estimate of heterogeneity. Determine which sampling design best accommodates the spatial and temporal boundaries of the population.

9.2.1.2 Subdivision of the site may involve spatial boundaries such as drums, tanks, an area within a grid, a boring location on a grid, a depth interval in a boring, distance along

a conveyor belt, or any other appropriate defined physical unit from which material can be obtained. For example, a defined search area may be the answer to locate an 8–ft diameter area of PCB contamination from a 55–gal drum PCB spill.

9.2.2 *Determine Optimum Number of Samples*:

9.2.2.1 Budgets and the acceptable levels of uncertainty as defined by the DQO or project objective planning process are competing factors that affect the number of samples. Statistical techniques for balancing these competing factors are discussed in a number of places in the literature[6] and Appendix X1.

9.2.2.2 The following illustrates a calculation for the commonly used systematic grid sampling and the iterations which may be necessary, if the calculated number of samples should prove, for practical reasons, to be too large to implement.

9.2.2.3 *Example Calculation*—The number of samples to be collected can be calculated based on variance information derived from previous sampling data or estimated based on professional judgment. Usually the contaminants of concern (COCs)s are parameters which are closest to or in excess of an action level. Their presence is normally the driving force behind the need to determine the extent and levels of contamination. The statistic of interest here is the mean and it assumes a normal distribution.

(1) Select a margin of error (*p*) acceptable for the subsequent use of the data. For soil studies, a margin of error of 0.20 is not unusual. The margin of error may be calculated by dividing the needed precision, in units of concentration, for example, = 10 ppm, by the known or anticipated mean concentration of the COCs. Note, that if the actual precision or mean concentration for the COC differs from those estimated during the planning process, a re-evaluation of the assumed margin of error may be necessary.

(2) A coefficient of variation (CV), which is defined as the standard deviation of a COC divided by the mean of the COC, is either obtained using previous sampling data, or estimated based on anticipated variability. If a CV above 0.65 is obtained, a large number of samples will usually be needed to make a decision with the selected margin of error.

(3) A confidence level 100(1-α) % needs to be established. For work involving hazardous wastes, a confidence level of 95 % is frequently used. For a 95 % confidence level, using a standard *Z* statistical table, this corresponds to a one-sided statistical factor of $Z_\alpha = 1.645$.

(4) If a 1-sided inference about the population is desired (for example, comparing a mean concentration to a regulatory threshold), the required number of samples is calculated using the following formula:

$$n = \{Z_\alpha\ (CV)/P\}^2 \tag{1}$$

where:

n = number of samples to collect,
Z_α = statistical factor for the desired confidence level,
CV = coefficient of variation, and
p = margin of error.

In a case where no previous sampling data is available, the values used in the above discussion can be used as a starting point.

$$n = \frac{(1.65)^2(0.65)^2}{(0.20)^2} \tag{2}$$

$$n = 29 \text{ samples} \tag{3}$$

If a two-sided inference is desired (for example the mean is equal to 10 ppm), the *Z* value of 1.96 is used in the formula, instead of 1.65. The result is an n=40.

(5) Upon completion of the calculation the number of samples and the margin of error is reviewed to determine that each is acceptable. If the value of *n* number of samples is too great, then an adjustment to the margin of error should be considered, or the sampling design may be modified. Alternately, if the population is stratified by concentration, the number of samples required may be reduced by selecting a sampling design for each of the strata. The inter-strata variability would then be removed from the calculation of the needed number of samples.

(6) Table 1 illustrates the number of samples required at a 95 % confidence level (*Z*-table factor of 1.65) with varying margins of error (*p*) and coefficients of variation (CV).

(7) Note that as the CV increases at a set margin of error, the number of samples required increases. When the variability is low (as measured by the standard deviation or the square root of the variance) relative to the mean of the data, then the CV is low. However, as the variability in the population begins to increase relative to the mean of the data, then the CV increases and the number of samples required increases if characterization of the site at a 95 % confidence level and a set margin of error is desired.

(8) A similar relationship is observed for the margin of error. When the precision required (say ± 10 ppm lead) is high, relative to the mean of the data (say 100 ppm lead), then the margin of error is low (in this case 0.1). In this case 115 samples would be required with a CV of 0.65. If the investigators could accept a higher margin of error (for example, ± 20 %), and the mean concentration of the data is still 100 ppm lead, then the resulting margin of error (0.2) would result in a lower number of required samples. Note that 29 samples would be required at the same CV of 0.65 and a one-sided inference.

(9) If the confidence level is decreased to 80 %, then the required number of samples reflected in this figure would be lower for each margin of error and CV combination. However, the confidence level may fixed. One alternative to analyzing the larger number of samples may be to use compositing.

TABLE 1 Number of Samples (*n*) for given Coefficient of Variation and Margin of Error

	Coefficient of Variation (CV)				
	0.1	0.5	0.65	1.0	2.0
Margin of Error (*p*)					
0.1	3	68	115	272	1089
0.2	1	17	29	68	272
0.3	-	8	13	30	121
0.5	-	3	5	11	44
1.0	-	1	1	3	11
2.0	-	-	-	1	3

[6] Gilbert, R. O., *Statistical Methods for Environmental Pollution Monitoring*, Van Nostrand Reinhold Co., New York, 1987.

9.2.2.4 *Site/Event Considerations*—The site and physical sampling event(s) constitute the majority of the practical aspects to be evaluated. Each design should be evaluated against all practical aspects to determine whether or not a given design will be practical to implement. This evaluation is subject to professional judgment as to whether or not a practical aspect, for example, the level of personnel training needed, is practical or acceptable, or both. If it is not, then the design needs to be modified or eliminated. These aspects include, but are not limited to the following:

(1) Site Access and Conditions —Site considerations - cross contamination potential; limits on access to sampling locations (for example, buildings, refusals).

(2) Equipment and Personnel —Equipment limitations; experience of the field sampling team; experience of the analysts; field and laboratory resources.

(3) Sampling Event —Special site concerns (for example, unexploded ordnance); special analytical needs (for example, low level analyses, dioxin); special analytical concerns (for example, interferences, multiple phases, incompatibility); health and safety considerations; resistant matrices (for example, solidified material); investigation derived waste (IDW) generation.

(4) Schedule —Transitory events (for example, start-up, shut-downs); potential impacts on project schedule.

(5) Safety Considerations.

9.3 *Statistical and Cost Evaluation*—Following the evaluation of each sampling design for the practical considerations, there should be a reduced set of design candidates. At this point, the statistical aspects (for example, uncertainty) and estimated costs should be calculated in preparation for the final review by the decision makers. The types of calculations and the degree to which statistics are needed will be dependent on the project objectives. The statistical evaluation routinely addresses issues of false positive or negative error, accuracy and precision, representativeness, and objectivity versus subjectivity.

9.3.1 *Statistical Considerations*—Statistical evaluation techniques are numerous and discussed in a number of places in the literature, including ASTM and USEPA guidance documents. The degree to which the statistical evaluation needs to be employed depends on the project objectives. Routinely, the statistical evaluation includes the acceptable limits of the potential sampling and analytical error and any mechanisms established for their controlling. The following are some general guidelines.

9.3.1.1 *Sensitivity Analysis*—A sensitivity analysis will determine how each design performs when the underlying assumptions about the sampling activity are modified. Typically, this involves changing specific parameters within some reasonable range and establishing how each of these changes influences the expected decision error rates. A statistical power curve is a useful statistical tool used to evaluate whether a sampling design has the ability to meet the project objectives.

9.3.1.2 *Hypothesis Test*:

(1) Each statistical sampling design should include a statistical hypothesis test. A statistical model should be developed which describes the relationship of the measured value to the "true" value. This mathematical formulation clarifies how data generated from a design is to be interpreted and processed in testing the hypothesis. A tentative analytic form for analyzing the resulting data (for example, a student's *t*-test or a tolerance interval) should be specified in the project objectives. This information can be used to determine the minimum sample size which satisfies the project objective's limits on decision error.

(2) The objectives of a statistical design are to limit the total error, which is a combination of sampling and measurement error, to acceptable levels. Traditional laboratory methods tend to minimize measurement error, but can be so expensive that only a limited number of samples can be analyzed within budget. The advantage to using less precise methods which are relatively less expensive, is that it allows a significantly larger number of samples to be collected and analyzed. This may trade off an increase in measurement error for a decrease in sampling error. If so, given the natural variability in many environmental studies, this approach may reduce overall costs while limiting the total decision error rates to acceptable levels.

(3) Appendix X2 provides an example approach for a statistical treatment of the choice of an analytical method based on the analytical variance and the analytical cost per sample.

9.3.1.3 *Error Statements*—When authoritative or non-statistical designs are used, quantitative statements about data quality are limited to the measurement error component of the total study error. A statistical approach would allow a quantitative statement about the sampling error component of the total project error to be made and allow for determining the probability of making a decision error regarding the overall sampling event.

9.3.1.4 *Comparison of Sampling Designs Based on Statistical Considerations*:

(1) When Population Concentration Distribution is Random —When there are no trends, stratification or spatial correlation in the distribution of the contaminant concentration over an area, systematic grid and simple random sampling are usually equally precise.

(2) When Population Concentration Distribution Has Trends —In general, systematic grid sampling is more precise than simple random sampling and is less precise than stratified random sampling (in the estimation of the population mean), assuming strata are appropriately identified.

(3) When Population Concentrations Are Spatially Correlated —Spatial correlation refers to the fact that the concentrations of two samples taken in close proximity tend to be similar or correlated and that this correlation decreases as the distance between the two samples increases. Often, the presence of spatial correlation or clustering can be minimized by taking samples spatially far apart. A grid design and geostatistical data analysis may be used to eliminate the error associated with a random design. However, random sampling is useful in order to avoid human bias and is the design of choice when too little is known to stratify or grid. If the site has known differences due to the historical insult, fate, and/or transport of the pollutants, then this knowledge can best be used by a stratified design. Stratified random sampling will generally be more precise than simple random sampling.

9.3.2 *Cost Estimates*—Development of an estimate of the total cost of sample collection and analysis for each design option enables the decision team to compare the financial aspects of the sampling designs which meet the project objectives. These should include all aspects of the sampling design and analytical event(s). The cost differential between the alternate designs will frequently although not always, be closely related to the number of samples required. Detailed examples of cost estimates are included in USEPA's Guidance on DQO's (Appendix B).

10. Final Selection

10.1 The decision team should now have all the information needed to make a final selection of the most resource-effective design. The information is presented to the decision maker(s). The final comparison or evaluation may take the form of 10.2 or 10.3.

10.2 *Risk versus Cost*—Here, risk is an estimate of the probability of an incorrect decision and its associated degree of hazard. Because usually, the lower the risk, the more the implementation will cost, the acceptable level of risk is at the discretion of the decision maker. Assuming that each design option presented meets the project objectives, the dynamics of the final decision are usually a balance between risk and cost, as displayed in Fig. 5. The objective is to minimize the cost or risk, or both, relative to the project constraints (for example, false positives, false negatives).

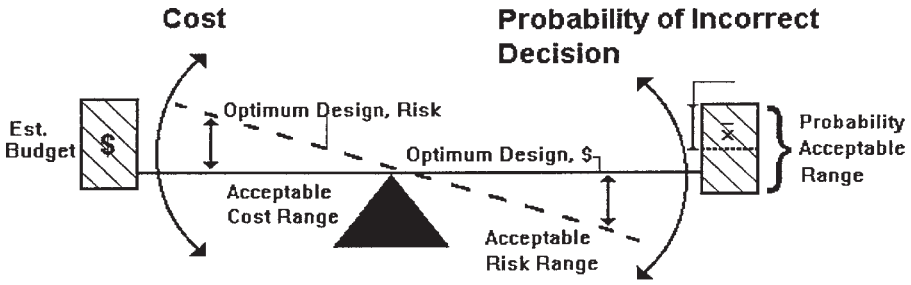
10.3 *Confidence Level versus Cost versus Time*—The balancing of the confidence level, cost and time constraints is shown in Fig. 6. Design modifications to achieve the needed balance can include: (*1*) an increase or decrease in the number of samples; (*2*) use of design tools such as compositing; (*3*) satisfying practical limitations; (*4*) a change in the study boundaries; (*5*) an increase in the tolerable design errors; (*6*) a relaxation of project constraints; or (*7*) modifications in the initial hypotheses.

10.3.1 Significant changes to one or more of the alternate designs would require that the optimization process be repeated, with a review of the potential practical constraints, re-calculation of the number of samples, re-development of the statistical and cost estimates, and a final review by the decision maker.

10.4 *Final Selection Options*:

10.4.1 Using the information generated to compare cost, risk, confidence level, time constraints and any other pertinent data, the decision maker can either (*1*) choose a sample design, or (*2*) reject the candidate designs.

10.4.2 If no design satisfactorily meets the requirements of the project objectives, including budgetary constraints and acceptable level of risk/error, then the sampling design or the project objectives will need to be modified. The design team should discuss with the decision maker whether modifications to the project objectives or the design option(s) are the most appropriate.



Dynamics of Design Optimization
(as cost increases risks decrease)

FIG. 5 Design Optimization

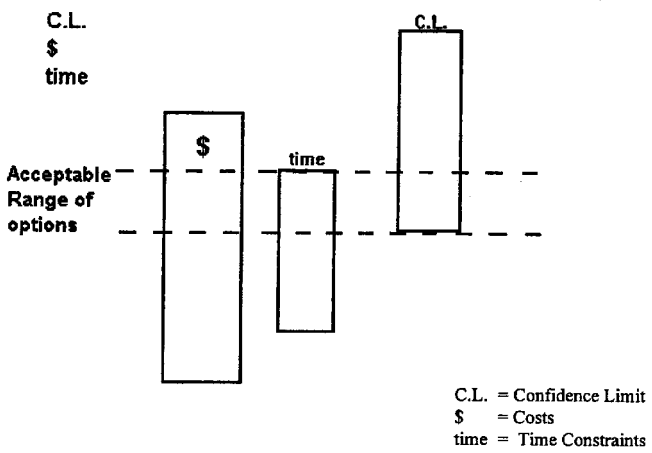


FIG. 6 Decision Variables

ANNEX

(Mandatory Information)

A1. COMMONLY USED SAMPLING DESIGNS

A1.1 Commonly Used Sampling Designs

A1.1.1 This section lists some of the commonly used sampling designs in environmental applications, with an explanation on their uses, advantages and limitations. The sampling designs discussed here include: authoritative sampling, simple random sampling, stratified random sampling, and systematic sampling. Each sampling design can be used alone, in combination with each other, or in combination with sampling design tools (see Section A1.2) such as compositing. Tables A1.1-A1.3 are a summary of the sampling designs and tools for quick reference.

A1.1.1.1 *Authoritative Sampling*—Authoritative sampling implies that some subjective human judgment is involved in the selection of the sampling location(s). There are generally

TABLE A1.1 Commonly Used Sampling Designs: Summary

Sampling Design	Uses	Advantages	Limitations
Authoritative			
Judgment	1-estimate of population mean 2-when population homogeneous 3-when high margin of error acceptable 4-when sampling designer knowledgeable	1-cost effective	1-if population heterogeneous, mean not easily estimated 2-has high margin of error 3-poor estimate of variance
Biased	1-ID localized contamination 2-Determine non-compliance	1-cost effective	1-cannot generalize to the entire population
Simple Random	1-when population not stratified	1-simple 2-estimates variance	1-if stratified populations, may not estimate mean accurately 2-need more samples 3-may not be easy logistically
Stratified Random	1-when population can be divided into relatively homogeneous strata	1-when resultant strata are homogeneous 2-representative samples 3-estimates variance	1-may be difficult logistically 2-strata must correctly reflect any contaminant stratification
Systematic Line Space Random	1-locate hot spots 2-map trends	1-samples easily identified and collected 2-can define contamination patterns 3-more accurate estimate of mean concentration	1-unrecognized trends or cycles may cause poor accuracy or precision, or both
Search	1-locate hot spots	1-cost effective 2-minimum samples needed 3-easy to implement	1-hot spot may be undetected
Unequal Probability	1-heterogeneous population 2-contaminant expected in specific fraction	1-more precise estimate of the chemical contamination in a heterogeneous material. 2-less costly	1-unrecognized trends or cycles may cause poor accuracy or precision, or both

TABLE A1.2 Sampling Design Tools: Summary

Sampling Design	Uses	Advantages	Disadvantages
Compositing	1-mean estimate of population 2-where optimum number of samples high	1-reduce inter-sample variance 2-reduce costs 3-determine presence/absence of hot spots	1-loss of volatiles during mixing 2-when cannot be properly mixed 3-when analytical costs low relative to sampling costs
Particulate Material Method	1-heterogeneous material mixture of granular material	1-statistical and defensible	1-very large sample size needed (exceeding the limit of the some field and most laboratory equipment)
Geostatistics	1-where need isoplath maps 2-where data collected on a spatial network	1-maximizes use of available data 2-modeling	1-highly specialized math modeling 2-subjective
Sequential: Formal or Wald	1-as a contributing information source 2-subsidiary to other methods	1-use minimum number of data points 2-cost effective	1-decisions restricted by formal rules 2-not allow for alternatives, value judgments, etc.

TABLE A1.3 Combination Sampling Design: Summary

Sampling Design		Advantages	Disadvantages
Phased Sampling	1-where screening and then confirmation appropriate 2-verification of screening	1-cost effective (field screening)	1-increased turn-around time of the project sampling phase
Sequential	1-informal approach is acceptable	1-reduced cost by initially undersampling, and adding additional samples as needed	1-unrecognized trends or cycles may cause poor accuracy or precision, or both 2-action alternatives need to be carefully defined

two kinds: judgment sampling and biased sampling. However, these sampling methods are not haphazard sampling, implying that any sampling location is acceptable. When used properly, these sampling schemes can be highly cost-effective. However, in authoritative sampling, no objective probability of selection is assigned to any of the units in the population. As a result, there is usually no way to estimate the sampling variance of the population.

A1.1.1.2 *Judgment Sampling*—In judgment sampling, the sampling location(s) is selected because it is deemed to be representative of the average conditions of the population. The sampling objective here is to obtain a quick, inexpensive sample(s) so that an estimate of the general (average) conditions of the population can be obtained. More than one sample can be taken to increase the confidence in the estimate of the population developed from the sample data.

(1) Uses —(*1*) When an estimate of the population mean is needed quickly and inexpensively, (*2*) when the population is relatively homogeneous, (*3*) when there is a high tolerable margin of error in developing a view of the population, or (*4*) when the sampling individual or design is knowledgeable and a good judgment can be made as to where to take the samples.

(2) Advantages —(*1*) May be quick and inexpensive, particularly if no re-sampling is needed.

(3) Limitations —(*1*) When the population is highly heterogeneous and more statistically based results are needed, its average conditions may not be easily estimated. (*2*) When the tolerable margin of error is small, this method cannot be used, unless the population is relatively homogeneous or more samples are taken. When too many samples are needed, its advantage in cost may disappear and its disadvantage in accuracy (absence of bias) and precision over other sampling designs may begin to rise. (*3*) The sampling variance calculated from "judgment" samples may not be a good estimate of the true population sampling variance.

A1.1.1.3 *Biased Sampling*—In biased sampling the objective is usually to detect the presence of contamination or to obtain a "worst case" sample. The sampling location(s) is selected based on available information or knowledge, especially in terms of visually contaminated areas or knowledge of contamination.

(1) Uses —(*1*) Detecting the presence of localized contamination, identifying the source of contamination, or determining non-compliance.

(2) Advantages —(*1*) Cost-effective for the intended purposes.

(3) Limitations —(*1*) Local detection of contamination from this method cannot be generalized to the entire site area or population. (The question of degree or extent of contamination in the entire population cannot be answered with this kind of sampling.)

A1.1.2 *Simple Random Sampling*—Simple random sampling considers all units in the population equally (see also A1.1.3 and A1.1.4). In this sampling scheme, all the units in the population have equal probability of being selected as one of the samples, and the selection of one sample does not affect the selection of the remaining samples. An appropriate number of samples are randomly collected from that population.

A1.1.2.1 *Uses*—(*1*) When potential personal bias needs to be minimized; (*2*) when the population has no identified patterns of contamination, such as stratification.

A1.1.2.2 *Advantages*—(*1*) This is the most simple random sampling design. Because the sample selection is based on probability, a representative set of samples can be expected and the sample data can be used to obtain an estimate of the population variance.

A1.1.2.3 *Limitations*—(*1*) If patterns or stratification exists, it may not provide an accurate (in both bias and precision) estimate of the population characteristic. (*2*) A large number of samples may be needed in order to achieve the desired level of precision in estimating the population characteristics (especially when the population is highly heterogeneous). (*3*) Logistically, it may not be easy to take samples at the specified random locations.

A1.1.3 *Stratified Random Sampling*—In stratified random sampling, the population is divided into non-overlapping subgroups (in space or time) called strata, where the contaminant concentration is similar within a stratum and dissimilar between the strata. Sampling locations are selected using simple random sampling within each stratum. One can also use a systematic design in each stratum. An overall estimate of the population characteristic (for example, mean concentration) is the weighted average of the stratum means, the weights being the relative sizes of the strata. The relative size of a stratum is defined as the ratio of the size of a stratum to that of the entire population.

A1.1.3.1 *Uses*—(*1*) When a population can be divided into different strata, especially when the stratification boundaries are consistent with the contaminant concentration, such that each stratum is relatively homogeneous relative to the characteristic of interest.

A1.1.3.2 *Advantages*—(*1*) If the division of the population into strata creates relatively homogeneous strata, this design will obtain a more accurate estimate of the population characteristic(s) than simple random sampling, using the same number of samples. (*2*) A representative set of samples can be obtained. (*3*) Sampling variance can be estimated.

A1.1.3.3 *Limitations*—(*1*) Collecting samples at random locations within a stratum may not be easy to implement logistically. (*2*) Greater accuracy/precision is probable only if the known stratification correctly reflects the strata, with maximum between-strata variability and minimum within-strata variability. (*3*) If each stratum is used as a unit upon which decision is to be made, then each stratum can be viewed as a population and a simple random sampling design can be used for each stratum.

NOTE A1.1—It is often desirable to have a more uniform distribution of the sampling locations throughout the population than a simple random sampling design. In such cases (for example, when sampling along a line or over an area), the population can be divided into blocks of equal or unequal sizes. These blocks can be construed to be "arbitrary" strata. These arbitrary strata can be defined by topography, political boundaries, or physical demarcations such as roads and rivers. A set of random or systematic samples can then be taken from within each block.

A1.1.4 *Systematic Sampling*—Systematic sampling involves the collection of samples at predetermined, regular intervals, in space or time. However, this method of sampling does not preclude the incorporation of random elements. Several of the commonly used designs will be discussed here.

A1.1.4.1 *Uses*—(*1*) These designs are applicable when there is a need to obtain samples more uniformly located throughout the population, as when a population is essentially random or contains a minimum of strata. (*2*) Identification of hot spots. (*3*) Mapping distribution of contaminants.

A1.1.4.2 *Advantages*—(*1*) It is relatively easy to identify the samples for collection and to implement under most field conditions. (*2*) It may be useful for defining patterns of contamination (trends or cycles). (*3*) In many cases, it will produce a more accurate estimate of mean concentration. (*4*) Particularly useful in detecting hot spots.

A1.1.4.3 *Limitations*—(*1*) Care needs to be taken so that the sampling locations do not coincide with unsuspected patterns or periodicity in contaminant concentration. Such coincidence may produce biased estimate. (*2*) An accurate estimate of the population sampling variance may be difficult.

A1.1.4.4 *Sampling Along A Line*—When sampling over a time or along a physical line, for example, a ditch, samples can be taken on a predetermined, regular interval along the line. Once the number of samples to be collected (*n*) is known, the sampling interval in space or time (*k*) can be determined.

$$k = N/n \tag{A1.1}$$

where:

N = is the total length of the line, and
k = is determined to the nearest integer.

One way to obtain the n samples is as follows: (*1*) picture the total length of the line (*N*) as extending around a circle (*2*) choose a random number between 1 and *N* as a starting point and (*3*) select every kth sample around the circle, until *n* of them have been obtained. This will provide a set of samples from which an unbiased estimate of the mean concentration can be determined.

A1.1.4.5 *Sampling Over Space (Square Grid)*—The most simple grid sampling design is a square grid design. One step wise procedure is:

(1) Calculated grid size G as $G = \sqrt{(A/n)}$, where A = area size, n = number of samples needed.

(2) Select an initial random point in the area.

(3) Construct coordinate axes going through the initial point.

(4) Construct lines parallel to the vertical axis, separated by grid distance *G*.

(5) Similarly, construct lines parallel to the horizontal axis.

(6) Locate sampling points at grid line intersections or at the center of grid cells within the site boundary.

(7) The total number of samples identified on the grid may be different from the number *n* which are needed. At this point, the several options include: (*a*) Taking all the samples identified on the grid, (*b*) taking only *n* samples out of the total located, *n* being based on best judgment, (*c*) taking samples at a random location in the grid squares, and (*d*) compositing the samples taken from within grid cells.

NOTE A1.2—There are many variations of this design. However, they offer essentially the same advantages and limitations.

A1.1.4.6 *Systematic Random Sampling*—Systematic random sampling is applied to a population by choosing a random starting time or location with the aid of random number tables or random number generator. The initial starting point is where a grid of equally spaced sampling locations is initiated. A second random number can be chosen to determine the orientation of the grid over the population. The grid dimensions or the distance between sampling locations is often determined by the budget which will determine how many

samples can be collected and analyzed. The sampling process is greatly facilitated by the fact that field personnel can easily measure to adjacent sampling locations. The fact that the first location and the grid orientation are chosen in a random manner ensures that operator bias does not impact the choice of sampling locations.

(1) Uses —(*1*) Where a uniform coverage of the site is needed.

(2) Advantages —(*1*) Detects concentration trends over time and space and under certain circumstances can yield a more accurate estimate of mean concentration. (*2*) Can be applied to a temporal population (for example, a wastewater effluent).

(3) Limitations —(*1*) Substantial bias can result if unknown concentration cycles coincide with the systematic sampling locations. Therefore historical or waste generation information is recommended to determine the likelihood of cyclic patterns in the population. (*2*) Inaccurate variance estimates occur when the concentration distribution is not random (for example, the systematic collection of samples crosses different strata) or if concentrations are serially correlated. (*3*) Substantial number of samples are required.

A1.1.5 *Search Sampling*—Search sampling is a strategy to increase the likelihood that at least one sample coincides with any existing areas of high concentrations or "hot spots." This involves (*1*) the estimation of the likely shape and size of the hot spot, and (*2*) the determination of the acceptable risk of not detecting the hot spot. With this information, the shape of the sampling grid units (for example, square or triangular) are chosen and the distance between sampling locations is calculated. The sampling locations may form a grid pattern similar to that of systematic random sampling.

A1.1.5.1 *Uses*—(*1*) To locate hot spots.

A1.1.5.2 *Advantages*—(*1*) This design provides for the maximum use of any knowledge of the site or location, or both. (*2*) Cost effective. (*3*) Minimum number of samples needed. (*4*) Ease of implementation.

A1.1.5.3 *Limitations*—(*1*) If the assumptions are incorrect, it is possible that a hot spot will exist between the sampling locations and remain undetected.

A1.1.6 *Unequal Probability Sampling*—Unequal probability sampling is similar to simple random sampling, except that a rule is used to unequally weight the likelihood that a given sample will be included in the data set. The samples to be included or excluded may be chosen based on a specific area of the strata, the size of the group or population, or the particle size of the waste.

A1.1.6.1 *Uses*—(*1*) To sample heterogeneous materials in which the contaminant of interest is expected to be found in a particular particle fraction, for example, the fines. The remaining items, for example, the large particles, can be ignored as part of the sample collected.

NOTE A1.3—It may still be necessary to know the mass of the large particles, depending on the project objectives.

A1.1.6.2 *Advantages*—(*1*) For a given number of samples of specific size, it often provides a more precise estimate of the chemical contamination in a heterogeneous material (than simple random sampling). (*2*) This design is less costly because fewer samples are needed for a given mass of waste.

A1.1.6.3 *Limitations*—(*1*) Poor accuracy and precision can occur when unrecognized trends or cycles occur in the population.

A1.2 Sampling Design Tools

A1.2.1 *Sample Compositing*—The compositing or combining of individual samples to form a composite sample is a mechanism to reduce the analytical costs, where a mean estimate value is either acceptable or the objective. The main physical issues to address are whether the individual sample matrices are compatible and how many samples it is appropriate to composite. See Guide D 6051. For example, if the regulatory limit is 50 ppm and the detection limit is 5 ppm, no more than 10 samples may be composited together in order to detect the possibility of a single sample exceeding the regulatory level of 50 ppm.

A1.2.1.1 *Uses*—(*1*) Where sample collection is inexpensive but analysis is costly. (*2*) Less than 20 % of the results are expected to exceed the blank values. (*3*) The objective is a mean estimation of the population.

A1.2.1.2 *Advantages*—(*1*) Reduce inter-sample variance; (*2*) reduce costs for estimating a total or mean value, especially where analytical costs greatly exceed sampling costs; (*3*) efficiently determine the absence or possible presence of hot spots or hot containers and, when combined with retesting schemes, identifying hot spots, as long as the probability of hitting a hot spot is low; (*4*) situations where the nature of the contaminant distribution tends to be contiguous and non-random and the majority of analyses are "non-detects" for the contaminant of interest; (*5*) provides a degree of anonymity where population, rather than individual statistics are needed.

A1.2.1.3 *Limitations*—(*1*) Loss of volatiles during mixing; (*2*) when the composite sample cannot be properly mixed and subsampled or the whole composite sample cannot be analyzed; (*3*) when the goal is to detect hotspots and a large proportion of the samples are expected to test positive for an attribute; (*5*) when analytical costs are low relative to sampling costs (for example, insitu field portable X-ray fluorescence takes only 30 s with no sample preparation so analytical costs/sample are very low; (*6*) when regulations specify that a grab sample must be collected.

A1.2.2 *Particulate Material Method*—The particulate material method is statistically based and extends into sample preparation. It seeks to provide an overall framework for sampling design, whereas, traditional random sampling schemes address only the statistical aspects of sample identification and data computation, leaving the question of particle size and sample volume to the chemist. This method was developed for the mining industry to sample ore. Characterization of ore is dependent on the sample volume, particle size, the degree of particle size reduction and the information available about the ore.

A1.2.2.1 *Uses*—(*1*) For sampling heterogeneous mixtures of granular material.

A1.2.2.2 *Advantages*—(*1*) The advantage to using this method is the defensibility afforded by the statistical approach.

A1.2.2.3 *Limitations*—(*1*) Extraordinarily large sample volumes may be required. Most laboratories cannot handle such

volumes and the aliquots used for environmental analytical methods make the sample volume unrealistic.

A1.2.3 *Geostatistic Sampling*—Geostatistic sampling includes techniques such as kriging and conditional simulation. Preliminary or exploratory study data can be used to optimize a sampling design where geostatistical data analysis methods are to be used. Statistically, conditional simulation techniques assume that the population is treated as though it is a realization of a random process: the population is random and the sample is deterministic. In other words, because the population is truly random, the sample locations may be selected subjectively rather than randomly. First, assumptions are selected and the population is mathematically modeled. Then from data or past experience one estimates a function which describes the spatial interrelation within the population, which is often subjectively selected when there is little available information. As data is obtained, the estimates are updated to provide final answers which are based on the most up-to-date co-variance estimates.

A1.2.3.1 *Kriging* is a technique in which a weighted moving average method is used to interpolate values from a sample data set onto a grid of points for contouring. It can be used to identify areas of high uncertainty and guide additional sampling. Kriging provides an unbiased estimate (minimizing the expected-square-error) of the average of a given attribute over a specified spatial region of the population. The method varies depending on the assumed statistical structure of the population and the attribute(s) to be estimated.

A1.2.3.2 *Conditional simulation* techniques use detailed computer simulations of a population, consistent with available data and assumptions of the population's statistical structure and spatial interrelations. Multiple simulations can be produced to demonstrate the degree of variability following collection of a suite of data points. This provides valuable information in determining future sampling locations or possible responses to remediation action, consistent with the current available data. If this shows too much variation, then more data should be collected.

(1) Uses —(*1*) Site assessment and monitoring situations where data are collected on a spatial network of sampling locations; (*2*) where contour maps of pollutant concentration (or other variables) are desired; (*3*) when sample collection and analysis are costly and it is necessary to maximize the information from each data point.

(2) Advantages —(*1*) These methods maximize use of the available data.

(3) Limitations —(*1*) These techniques are subjective. Judgment, experience, and skill are important factors.

A1.2.4 *Formal or Wald Sequential Testing*—In formal sequential testing, a hypothesis is developed; samples are collected and analyzed; and the data is used in a formal hypothesis test procedure with three possible actions: (*1*) accept the null hypothesis; (*2*) reject the null hypothesis; (*3*) insufficient data, collect additional samples. A formal stopping rule is used to determine which of the three actions is most appropriate.

A1.2.4.1 *Uses*—(*1*) Primarily as a contributing source of information for a practical decision process. (*2*) As a subsidiary to other methods.

A1.2.4.2 *Advantages*—(*1*) Action levels are reached with a minimum number of data points.

A1.2.4.3 *Limitations*—(*1*) The formal procedures restrict the decisions made by not allowing for the alternate courses of action, value judgments, etc.

A1.3 Combination Sample Designs

A1.3.1 The following are frequently used sampling designs which combine any of the above discussed designs, sampling tools and/or employ a multi-step sampling design. The uses, advantages and limitations will be the same as those of the primary design(s) or tools used.

A1.3.1.1 *Phased or Two Stage Sampling*—Phased sampling is a general term for a two step method using one or more of the previously discussed designs. A first set of samples is collected and analyzed. The resulting data is then used to design the collection and analysis of the second set of samples. Most commonly, a large number of samples is selected to be analytically screened, inexpensively. Based on the first sample results a second, smaller set of samples is selected, and analyzed with more precise, costly methods. With *random sampling* models, the first data set is used to obtain estimates of the population variance. This provides guidance for selection of the most appropriate number or location, or both, of the subsequent set of samples. With *geostatistical techniques* the first data set is chosen to estimate or verify the population intercorrelation or other structural population assumptions. The second data set provides the basis for least-cost computation of the estimates of the target precision.

(1) Uses —(*1*) Particularly useful for verifying field screening results using more rigorous methods. The closer the screening procedure correlates with more accepted/rigorous technique, the more acceptable the screening procedure. If the screening measurement is relatively inexpensive, a more accurate characterization of a waste site can be achieved by increasing the number of measurements.

(2) Advantages —(*1*) The principal advantage to this method is the cost reduction by using field screening methods, followed by fewer more precise and expensive, regulatory required sampling. (*2*) Using random sampling methods reduces the variance on the final samples because of the number of samples. (*3*) Geostatistical sampling provides for reduced costs and maximum information from each data point.

(3) Limitations —(*1*) The turn-around time of the sampling phase of the project is relatively long, because the sampling and analyses are performed twice.

A1.3.2 *Sequential Sampling*—This more informal sequential testing is an extension of double sampling and is not restricted to the formal Wald process. It includes aspects of sequential testing, allows decision making with minimal data and may be used with either random sampling or geostatistical techniques.

A1.3.2.1 *Uses*—(*1*) Where the more formal approach is not as critical.

A1.3.2.2 *Advantages*—(*1*) The sequential sampling approach reduces cost by initially under sampling then adding samples, as needed.

A1.3.2.3 *Limitations*—(*1*) The action alternatives, types of data needed at each stage, etc., need to be carefully defined.

APPENDIXES

(Nonmandatory Information)

X1. ADDITIONAL REFERENCES

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X2. CHOOSING ANALYTICAL METHOD BASED ON VARIANCE AND COST

X2.1 Choosing and analytical method based on the analytical variance and analytical cost per sample can be formalized through the following calculations. These are based on the comparison of two methods at a time.

Let s_i^2 = estimated analytical variance for method i,
c_i = analytical cost per sample for method i,
C_i = cost of analysis for n_i samples for the ith method $= n_i c_i$,
X_i = mean of n_i analyses for the ith method, and
i = 1 or 2 (representing the first or second method being considered).

X2.2 Equal precision between X_i and X_2 can be achieved by setting:

$$\text{Var}\,(X_1) = \text{Var}\,(X_2) \tag{X2.1}$$

$$s_1^2 \,/\, n_1 = s_2^2 \,/\, n_2 \tag{X2.2}$$

X2.3 Rearranging these equations yields:

$$n_1 = n_2(s_1^2/s_2^2) \tag{X2.3}$$

X2.4 Substituting for n_1, therefore creates the expression:

$$C_1 = n_1 c_1 = n_2(s_1^2/s_2^2)c_1 \tag{X2.4}$$

and dividing by $C_2 = n_2 c_2$ gives:

$$C_1/C_2 = (s_1^2/s_2^2)(c_1/c_2) \tag{X2.5}$$

X2.5 Given estimates $s_1{}^2$, $s_2{}^2$, c_1 and c_2, the ratio C_1/C_2 can be calculated. The optimal cost at an equal precision can be established by using the following:

X2.5.1 If $C_1/C_2 < 1$, choose method 1.

X2.5.2 If $C_1/C_2 > 1$, choose method 2.

X3. CALCULATING THE NUMBER OF SAMPLES: A STATISTICAL TREATMENT

X3.1 Summary of Calculations

Sample Design	Assumption	Equation No.
Simple Random Sample	Prescribed Precision	Eq X3.1
	Estimated Variance	Eq X3.2
	Prescribed Margin of Error Prescribed Precision	Eq X3.3
	Prescribed Margin of Error Estimated Variance	Eq X3.4
	Prescribed Margin of Error Prescribed Relative Error	Eq X3.5
	Specified False Positive and False Negative Errors	Eq X3.6 Eq X3.7
Stratified Random Sampling	Optimal Allocation of Samples to Strata	Eq X3.8-X3.11
	Total Number of Samples for Prescribed Fixed Cost	Eq X3.12
	Total Number of Samples for Prescribed Variance	Eq X3.13
	Total Number of Samples for Prescribed Margin of Error	Eq X3.14
Multi-Stage Sampling	Two Sources of Variation	Eq X3.16-X3.18

Search Sampling for Hot Spots	Hot Spots are Small Sizes	Eq X3.20
Grid Sampling for Hot Spots	Hot Spots of Defined Size and Shape	Eq X3.22
	Multiple Hot Spots	Eq X3.26
Composite Sampling	Estimation Problem	Eq X3.27-X3.30
	Classification Problem	Eq X3.33-X3.38

X3.2 How to Determine the Number of Samples

X3.2.1 Many of the following methods are described in footnotes 6 and 8. [6,8] Paragraph X3.2.2 describes the methods for calculating the number of samples needed for estimation of the population mean concentration, for simple random and stratified random sampling designs. Paragraph X3.2.3 describes multi-stage sampling methods when the objective is to statistically detect hot spots. The needed number of samples can vary according to site specific conditions (for example, degree of heterogeneity in the sampling materials) and specifications (for example, acceptable precision, false positive error and false negative error).

X3.2.2 *For Estimation of Mean Concentration*—This section assumes that the population is so large that it can be construed to contain an infinite number of sampling units or items.

X3.2.2.1 The formula for calculating the needed number of samples are often given for two cases: when the population variance is known and when the population variance is estimated. The population variance can be construed to be known when there is history or experience as to what the size of the variance is. When this is the case, the *z* statistic is used in the formula. On the other hand, if the population variance is estimated from certain data, then the *t* statistic is used instead. Oftentimes, the difference in the numbers of samples produced by the two different approaches do not differ very substantially.

X3.2.2.2 Since there is generally lack of data to estimate the population variance, the formula with the *z* statistic can often be used as an approximation. If high precision in the needed number of samples is required, then a pilot study to provide a good estimate of the variance may be called for.

X3.2.2.3 The methods also assumes little or no spatial correlation between the samples. Where appropriate, a one-sided inference about the population is assumed.

X3.2.2.4 *Sample Random Sampling*:

(1) For Prescribed Precision — The variance of the estimated mean concentration is a measure of precision. In many applications, it is often required that this variance be no larger than a prescribed value *v*. The number of samples needed in this situation is given below.

When the population variance σ^2 is known

$$n = \sigma^2/v \quad \text{(X3.1)}$$

where:

n = needed number of samples,
σ^2 = known population variance, and
v = prescribed size of the variance of sample mean Var (x).

When the population variance is estimated—When population variance is estimated from an initial set of n_1 samples to compute the variance s^2 as an estimate of the population variance σ^2, then:

$$n = (s^2/v)\,(1 + 2/n_1) \quad \text{(X3.2)}$$

(2) For Prescribed Margin of Error — When the absolute deviation of the sample mean from the true mean must be within a prescribed limit *d* with 100 (1-α) % probability. If the population mean is μ and the sample estimate is *x*, then $d = \bar{x} - \mu$.

When population variance is known

$$n = (z_{1-\alpha}\sigma/d)^2 \quad \text{(X3.3)}$$

where:

d = specified or acceptable absolute deviation of the estimate from the true value, or the absolute limit of error in estimation,
$1-\alpha$ = confidence level of not exceeding the prescribed margin of error d, and
$z_{1-\alpha}$ = the 100 $(1-\alpha)$ percentile point of standard normal distribution.

(3) The relationships among selected values of α, $z_{1-\alpha}$ and confidence level (for a one-sided inference about the population) are given below:

α	Confidence Level, %	$z_{1-\alpha}$
0.20	80	0.842
0.10	90	1.282
0.05	95	1.645
0.025	97.5	1.960
0.01	99	2.576

For a two-sided *z* value, simply multiply the α value by 2, re-calculated the confidence level as 100 $(1-\alpha)$, and then look for the corresponding *z* value. For example, the two-sided *z*-value with 95 % confidence is 1.96. Often a *z* value of 2 is used because of the uncertainty in estimating the standard deviation (σ).

When the population variance is not known and is estimated from *m* samples, then z in Eq X3.3 is replaced by *t*, resulting in Eq X3.4:

$$n = (t_{1-\alpha,m-1}s/d)^2 \quad \text{(X3.4)}$$

where:

[8] Cochran, William G., *Sampling Techniques*, 3rd ed., John Wiley and Sons, 1977.

$t_{1-\alpha,m-1}$ = the 100 (1–α) percentile point of the *t*-distribution with (*m*–1) degrees of freedom.

(4) For Prescribed Relative Error — Often a reliable value of σ^2 is not available but a coefficient of variation (CV) can be provided. In such cases, the margin of error in *(2)* can be specified as a percentage of the mean such that this relative error is no larger than a prescribed value d_r with 100 (1–α) % confidence. Thus,

$$n = (z_{1-\alpha}CV/d_r)^2 \quad \text{(X3.5)}$$

where:
CV = coefficient of variation in % = 100s/*x*,
d_r = relative margin of error in % = $100\,|\,\bar{x}\,|/\mu$, and
μ = population mean.

Eq X3.5 is useful because it is often easier to estimate CV than the variance σ^2.

(5) For Both False Positive and False Negative Errors —When it is desirable to estimate the number of samples needed for specified false positive error (typically denoted as α) and false negative error (typically denoted as β) for a decision rule, then the formula is:

$$n = (z_{1-\alpha} + z_{1-\beta})^2\sigma^2/\delta^2 \quad \text{(X3.6)}$$

where:
α = false positive error,
β = false negative error,
σ = population standard deviation, and
δ = deviation from the true mean important to detect.

Some example values of $z_{1-\alpha}$ and $z_{1-\beta}$ are given in the table in the previous section.

Eq X3.6 can be modified when the population variance is estimated by s^2, an approximate number of samples is:

$$n = (z_{1-\alpha} + z_{1-\beta})^2s^2/\delta^2 + (z_{1-\alpha})^2/2 \quad \text{(X3.7)}$$

The quantity δ in Eq X3.6 and X3.7 is a quantity which needs to be negotiated and agreed to. It often represents a departure from some reference value (such as regulatory limit) which is important to detect statistically. When it is large, the tolerance for departure from the reference value is high and the resultant number of samples required will be small. When it is small, the tolerance for departure from the reference value is low and the resultant number of samples required will be large. A balance in these considerations would lead to an agreed δ.

NOTE X3.1—It needs to be noted that when this method is used (Eq X3.6 or Eq X3.7), the number of samples required is in general much larger than the previous methods (for example, Eq X3.3-X3.5). The number of samples increases rather rapidly as the specified false negative error decreases.

X3.2.2.5 *Stratified Random Sampling*—This section describes the methods to determine the number of samples to collect from each stratum in stratified random sampling, for the purpose of estimating the mean concentration over all the strata. If the sampling objective is to estimate the mean concentration of each of the strata, then a simple random sampling design can be applied to each stratum.

(1) Optimal Allocation of Samples to Strata —If the sampling cost function is:

$$\text{Cost} = C = c_0 + \Sigma_{i=1,s}c_in_i \quad \text{(X3.8)}$$

where:
c_0 = fixed overhead cost,
s = number of strata,
c_i = cost of taking a sample from the *i*th stratum, and
n_i = number of samples to be taken from the *i*th stratum.

then the optimal allocation is to allocate n_i samples (of the total number *n* to be collected) to *i*th stratum as follows:

$$n_i = n\frac{w_i\sigma_i/\sqrt{c_i}}{\Sigma_{i=1,s}(w_i\sigma_i/\sqrt{c_i})} \quad \text{(X3.9)}$$

where:
n = total number of samples to be taken from all the strata, and
w_i = proportion of stratum i to the entire population (N_i/N).

If the cost of sampling is the same among the strata, Eq X3.9 reduces to:

$$n_i = n\frac{w_is_i}{\Sigma_{i=1,s}w_is_i} \quad \text{(X3.10)}$$

where:
s_i = standard deviation of samples from stratum *i* estimated from prior data.

A simple alternative to Eq X3.9 and X3.10 is proportional allocation. In this scheme,

$$n_i = w_in \quad \text{(X3.11)}$$

That is, if a stratum is *p* % of the population, then *p* % of the total samples will come from that stratum. For example, *p*=30 %.

The above equations requires the knowledge of *n*, the total number of samples *n* to take over all the strata. The sections below deals with this issue.

(2) Total Number of Samples for Prescribed Fixed Cost —When the total cost *C* is fixed, the optimal total number of samples is:

$$n = \frac{(C-c_0)\Sigma_{i=1,s}(w_is_i/\sqrt{c_i})}{\Sigma_{i-1,s}(w_is_i\sqrt{c_i})} \quad \text{(X3.12)}$$

where:
s_i = estimated standard deviation of samples from stratum i, and
$C–c_0$ = money available for sampling and analysis.

(3) Total Number of Samples for Prescribed Variance — If the variance of the estimated mean cannot exceed a prescribed value *v*, an approximation is:

$$n = \Sigma[(w_i^2s_i^2)/f_i] / [v + (w_is_i^2)/N] \quad \text{(X3.13)}$$

where:
f_i = sampling fraction from stratum *i* (or the proportion of total number of samples n to be taken from stratum *i*).

f_i in Eq X3.13 can be made identical to w_i.

(4) Total Number of Samples for Prescribed Margin of Error —If proportional allocation is used, then the optimal number of samples can be obtained for a specified (absolute) deviation of the estimated mean from the true value by no more than d with 100 (1–α) % confidence. An approximation is:

$$n = [Z^2_{1-\alpha}\Sigma_{i=1,s}w_i^2s_i^2/d^2] / [1+z^2_{1-\alpha}\Sigma_{i=1,s}w_is_i^2 / (d^2N)] \quad \text{(X3.14)}$$

When *N* is very large, Eq X3.14 is reduced to:

$$n = Z^2_{1-\alpha}\Sigma_{i=1,s}w_i^2 s_i^2 / d^2 \quad \text{(X3.15)}$$

X3.2.3 *Multi-Stage Sampling/Measurement Process*—Often a sampling and analytical plan consists of several stages of sampling and analysis, leading to multiple sources of variation. One objective here is to determine the optimal number of samples needed at each of the stages.

X3.2.3.1 The precision of the estimate of the population mean concentration often depends on, for example, the number of field samples, the number of laboratory samples and the number of analyses performed on each of the laboratory samples. In this example, the sampling stages include field, laboratory and analysis, leading to sources of variation from field sample variation, laboratory sample variation and "analytical variation." Note that the "analytical variance" here may not be the true analytical variance, depending on whether the split samples analyzed are identical or not. If the laboratory sample is homogenous, leading to identical splits, then the "anatical variance" component reflects the true analytical variance. If the splits are not identical due to laboratory subsampling, then the Analytical variance "component" above actually includes analytical variance and laboratory subsampling variance.

X3.2.3.2 A simpler example is the one above but without replicate analyses, where each laboratory sample is analyzed in total. In this case, there are two sources of variation: field sample to field sample (or between sample) variation and analytical (or within sample) variation.

X3.2.3.3 In any case, a mathematical model can be laid out to describe the sampling and analytical plan, by which these sources of variation can be estimated (called variance components of the total variation). This is an area where a statistician needs to be consulted, regarding the optimal design of the plan and the proper estimation of the variance components.

X3.2.3.4 In the simplest case of only two sources of variation (between sample and within sample), the standard deviation of the mean concentration from n samples, each analyzed r times, is:

$$\sigma_m = \sqrt{[\sigma_b^2/n + \sigma_w^2/(nr)]} \quad \text{(X3.16)}$$

where:

σ_m = standard deviation of mean concentration,
σ_b^2 = between sample variance,
σ_w^2 = within sample variance,
n = number of samples, and
r = number of replicate analyses for each sample.

And, as a result, the total cost of sampling and analysis is:

$$C_t = n(C_b + rC_w) \quad \text{(X3.17)}$$

where:

C_b = cost of obtaining a sample, and
C_w = cost of one analysis of a sample.

X3.2.3.5 Given Eq X3.16 and X3.17 and estimates of σ_b^2 and σ_w^2, one way to determine n and r is as follows:

(1) Specify an acceptable value of σ_m.

(2) Then, the optimal number of analyses per sample is:

$$r = (\sigma_w/\sigma_b)\sqrt{(C_b/C_w)} \quad \text{(X3.18)}$$

(3) The value of r from Eq X3.18 is substituted into Eq X3.16 to obtain the optimal value of n.

NOTE X3.2—Note that the calculated n and r are rounded up to the nearest integer.

(4) This approach is quite useful as it takes into account all the important sources of variations to determine the optimal combination of numbers of field samples, laboratory samples, laboratory subsamples, and laboratory analyses, and so forth. And this is part of optimization of the sampling plan.

X3.2.4 *Search Sampling: For Detection of Hot Spots*—Localized areas of high concentration are commonly called hot spots. Some examples of determining the numbers of samples for the detection of hot spots are given in this section.

X3.2.4.1 *When Hot Spots are of Small Sizes*:

(1) When hot spots are of small sizes, the number of samples needed for detecting at least one of them can be determined so that if none is detected there is little likelihood that any hot spots exist.

(2) If we let $x_1, x_2, \ldots, x_n$ be a set of n random sample from the population and assume that they are independent, then one way is to find this number of samples n such that we have high confidence (with 100(1–α) % confidence) that at least one hot spot will be detected. If p is the probability of the existence of a hot spot and this p is constant for all hot spots, then the probability of finding at least one hot spot is:

$$1 - (1-p)^n = (1-\alpha) \quad \text{(X3.19)}$$

Therefore, the number of samples needed in this case is:

$$n = ln\alpha/ln(1-p) \quad \text{(X3.20)}$$

where α is suitably small (for example, 0.05 or 0.10). The number of samples n for some values of p and α is given in Table X3.1.

X3.2.4.2 *Grid Sampling for Detecting Hot Spot of Defined Size and Shape*:

(1) Systematic grid sampling methods have been used in detection of hot spots of defined size and shape. For a defined target population, the intersections of the grid lines determine the number of samples to be taken. In general, the smaller the grid distance (the distance between two adjacent intersections)

TABLE X3.1 Number of Samples *n* as a Function of *p* and α (Eq X3.18)

α	*p*	*n*
0.05	0.05	59
	0.1	29
	0.2	14
	0.3	9
	0.4	6
	0.5	5
	0.6	4
	0.7	3
	0.8	2
	0.9	2
0.10	0.05	45
	0.1	22
	0.2	10
	0.3	7
	0.4	5
	0.5	4
	0.6	3
	0.7	2
	0.8	2
	0.9	2

is, the larger the number of samples is and the higher the chance of detecting a hot spot of a given size and shape.

(2) In general, triangular grid design seems to be superior to various patterns of square grid design, in terms of probability of detection.

(3) The following parameters need to be specified in order to determine the grid distance for detecting a circular or elliptical hot spot: (*a*) *L*, the length of semi-major axis of the hot spot (this defines the size of the hot spot); (*b*) *S*, ratio of the length of the short axis to the length of the long axis (this defines the shape of the hot spot); and (*c*) β, the acceptable probability of not finding the hot spot.

(4) A major axis is the long side of an ellipsoid. Semi-major axis is simply half of the major axis. In the case of a circular hot spot, the major axis equals the minor axis, which is the short side of an ellipsoid. The following discussions will focus on ellipitcal hot spot.

(5) Once these parameters have been specified, graphs[6] can be used to determine the grid distance *G*, which will leads to the numbers of samples needed.

(6) If the concentration defining a hot spot is higher than chemical method detection limit, then an alternative method is to define the size of the hot spot by the detection limit, instead of the original cutoff concentration for a hot spot. Since the detection limit is lower than the original cutoff concentration, the size of the hot spot is now larger and therefore a smaller number of samples is required to detect with the same probability of detection.

(7) This is equivalent to re-specifying *L*, the length of the semi-major axis of the hot spot using the detection limit, instead of the original cut-off.

(8) Namely, if the hot spot concentration limit is c_h and it is higher than the method detection limit c_d, then, for the purpose of detection, we can define the boundary of the hot spot by c_d, instead of c_h.

(9) The next thing to do is to determine the semi-major axis L* based on c_d, instead of *L* based on c_h. If $c_h > c_d$ and there is a gradient of declining concentration from the center of the ellipsoid outward toward the edge of the hot spot, then two potential solutions for finding *L** are:

(10) Asssuming Change in Concentration Is Inversely Proportional to Change In Semi-Major Axis —This assumption means that, as the semi-major axis moves from *L* to *L** (*L**>*L*), the decrease in concentration is inversely proportional to the length of the semi-major axis. Namely,

$$L^*/L = c_h/(pc_h) \quad \text{(X3.21)}$$

where:

c_h = hot spot concentration limit at the outer edge of *L*, and
p = c_d/c_h, $0<p<1$.

Thus,

$$L^* = L/p \quad \text{(X3.22)}$$

For example. Let $L = 50'$ and $p = 0.1$ (that is, c_d is only 10 % c_h). Then

$$L^* = 500' \quad \text{(X3.23)}$$

*L** can then be used to determine the grid distance, leading to a smaller number of samples than when *L* is used.

(11) Asssuming Change in Log Concentration Is Inversely Proportional to Change In Semi-Major Axis —This is similar to above, except that the assumed relationship is a logarithmic one. Namely,

$$L^*/L = ln[c_h/(pc_h)] = ln(1/p) \quad \text{(X3.24)}$$

Thus,

$$L^* = L[ln(1/p)] \quad \text{for } 0 < p < 0.36 \quad \text{(X3.25)}$$

where [1*n* (1/*p*)] is multiple factor of *L** relative to *L* (called here the multiplier effect). In order for this effect to be greater than 1, *p* needs to be smaller than 0.36. This effect as a function of *p* is given in Table X3.2.

(12) Other relationships can be postulated, in addition to those described in Eq X3.22 and X3.25. In place of detection limit, some other quantities such as $(c_h + c_d)/2$ can be considered as well.

(13) Since *L**>*L*, therefore the grid distance is increased, thereby decreasing the number of samples needed.

(14) The relationships between grid distance *G* and semi-major axis *L* are illustrated in Table X3.3.

(15) This method of reducing the number of samples by increasing the semi-major axis of the hot spot could lead to detection of larger number of "hot spots" based on c_d, which may not be hot spots at all based on c_h. Thus, this method is likely to be useful only when the target population is known to be relatively uncontaminated and the chance of false detection based on c_d is likely to be small.

(16) Once a hot spot based on c_d is identified, then either a field method or other sampling approaches can be used to further define the extent or boundary of the true hot spot of concern, namely the hot spot based on the original cut-off concentration c_h.

X3.2.4.3 *Multiple Hot Spots in Grid Sampling*:

(1) The grid distance determination in the section above is for detecting a single hot spot. When there are multiple hot spots, the grid distance can be determined for detecting at least one hot spot with a high degree on confidence. When none is detected, the probability of the existence of any hot spots can be expected to be very small. This is analogous to X3.2.4.1, except here the size and shape of the hot spots are considered in grid sampling.

(2) Again, in the determination of grid distance *G*, it requires specification of the following parameters:

L = length of semi-major axis of the smallest hot spot,
S = ratio of the short axis to the long axis of the hot spot, and
β = probability of not finding a hot spot of size *L* or larger when it actually exists.

(3) In the above definitions, β is the probability of not finding a hot spot. When there are multiple hot spots, under the simplifying assumption of equal size and shape, the probability

TABLE X3.2 Multiplier Effect Between *L* and *L (Eq X3.25)**

p	Multiplier
0.3	1.20
0.1	2.30
0.05	3.00
0.01	4.61

TABLE X3.3 Approximate Relationships Between Grid Distance *G* and Semi-Major Axis *L* in Circular Hot Spots

L (ft)	β	*G* (ft)
25	0.1	45
	0.2	49
	0.3	53
	0.5	63
50	0.1	89
	0.2	98
	0.3	106
	0.5	125
100	0.1	180
	0.2	196
	0.3	213
	0.5	250
200	0.1	357
	0.2	392
	0.3	426
	0.5	500
300	0.1	536
	0.2	588
	0.3	638
	0.5	750

of not finding any hot spots, for given β, is β^h, where *h* is the number of hot spots. As β is typically defined to be very small ($0<\beta<1$), β^h can become very close to zero as *h* increases, leading to very short and impractical grid spacing.

(4) One way to overcome this problem in the case of multiple hot spots is to set the probability of detecting at least one out of h hot spots to be the same as the probability of detecting a hot spot in a single hot spot case. From there, the corresponding β for determining the grid distance in the multiple hot spots case can be derived.

(5) Let it be given that $\beta=\beta_0$ for the single hot spot case. Then:

$$\text{Prob(detecting a hot spot } | h=1) = 1 - \beta_0$$

where *h* = number of hot spots.

(6) In the multiple hot spots case,

$$\text{Prob(detecting at least 1 hot spot } | h>1) = 1 - \beta^h$$

Let:

$$\text{Prob(detecting at least 1 hot spot } | h>1) = 1 - \beta_0$$

$$= 1 - \beta^h$$

Thus, the β to use to determine the grid distance for detecting at least one out of h hot spots is:

$$\beta^h = \beta_0 \quad \text{(X3.26)}$$

$$\beta = (\beta_0)^{1/h}$$

Thus, once the acceptable probability of not detecting a single hot spot is specified to be β_0, the value of β for the multiple hot spots case can be determined by Eq X3.26. We can then use this new β to determine *G*. Since $\beta>\beta_0$, the new grid distance will be larger than the one based on β_0, leading to smaller number of samples needed.

(7) For example, the originally specified probability of not finding a hot spot, β_0, may be 0.1. If there are h=4 hot spots, the new β is 0.56 ($= 0.1^{1/4}$). Because of this higher value of β, the grid distance *G* is increased accordingly.

(8) If this degree of increase in β is too steep, it can be modified, for example, by using $\sqrt{h}$ instead of *h*, in Eq X3.26.

(9) This approach seems reasonable in areas where no known contamination is present. For such areas, the sampling objective is to determine if some potential hot spots may be present. Thus, a sampling plan designed to detect, with high probability, at least one out of several potential hot spots seems to be a reasonable one. If the sampling plan fails to detect any, then the chance of presence of hot spots is small. On the other hand, if it does detect some hot spot(s), then more extensive sampling or field methods may be required to better define the areas of contamination.

(10) There is the issue of how the number of hot spots, *h*, is to be determined in the use of Eq X3.26. A reasonable approach is to assume that hot spots are associated with topographical depressions. In that case, the number of hot spots can be assumed to be the number of identifiable depressions.

X3.2.4.4 *Composite Sampling*—Composite sampling can be used in two broad areas. Both areas have potential of substantially reducing analytical costs. The two areas are: (*1*) Estimation of mean and variance with greater precision (in standard error of the mean). This is viewed as an estimation problem; and (*2*) detection of presence or exceedance in any of the samples in the composite. This is viewed as a classification problem.

NOTE X3.3—Since composite sampling has a wide variety of applications, a statistician can be consulted. This section describes some simple cases.

(1) Estimation Problem — A simple example of composite sampling is given below.

(2) Let *x* be a random variable representing the concentrations of independent and identical (same volume or weight) individual samples and *x* is normally distributed as $N(\mu, \sigma^2)$. Let y_k be the composite of *k* individual samples. Then it is known that y_k is an unbiased estimator of the population mean with greater precision because:

$$E(y_k) = \mu \quad \text{(X3.27)}$$

$$\text{Var}(y_k) = \sigma^2/k$$

if the composite sample is totally homogeneous. The factor *k* is greater than 1 by definition of compositing. In case *m* ($m>1$) composite samples are used for assessing attainment of cleanup standard, then:

y_m = mean concentration of m composite samples, each a composite of *k* individual samples
$= \Sigma y_{k,i}/m,\ i=1,2,\ldots,m$

Again, this mean of composite samples is unbiased with even greater precision than that observed by Eq X3.27, because:

$$E(y_m) = \mu \quad \text{(X3.28)}$$

$$\text{Var}(\bar{y}_m) = \sigma^2/(km)$$

(3) If we have an estimate of the variance of the individual samples σ^2, then we can find combination(s) of *k* and *m* which achieves some desired level of the variance (or the standard

deviation) of y_m. Some example reductions in the variance of the mean as a function of m and k, relative to the variance of individual samples, are given in Table X3.4.

(4) This kind of composite sampling can be applied to many other situations.

(5) In estimation, it is to be noted that, if only a subsample of the composite is analyzed chemically, then proper mixing to achieve homogeneity in the composite sample is important. In case when the composite sample is not totally or nearly homogeneous, then subsampling would introduce an additional source of variation, which may be called the heterogeneity variance σ_h^2. When σ_h^2 is not nearly zero, Eq X3.27 becomes:

$$\text{Var } (y_k) = \sigma^2/k + \sigma_h^2 \tag{X3.29}$$

and Eq X3.28 becomes:

$$\text{Var } (\bar{y}_m) = [\sigma^2/k + \sigma_h^2]/m \tag{X3.30}$$

(6) All the correct sampling and subsampling procedures must be followed to prevent biased results and assure reduction in sampling variance.

(7) On some occasions when analytical costs are high (relative to sampling costs), one composite sample may be used for inference purposes, especially when it is a composite of many individual samples. Since it is a composite of many samples, the concentration of the composite can be expected to have a much lower standard error than the individual samples. When this standard error is judged to be small, the concentration of the composite can be used for comparison against a standard or limit. This is especially appropriate when there is a pilot study to provide the relationship between the variances of the individual samples and the composite samples.

(8) Regarding questions such as the optimal number of individual samples needed in a composite, the number of composites, and subsamples of the composite and the like, a statistician needs to be consulted.

TABLE X3.4 Percent Reduction in Standard Deviation of Mean Concentration Estimate, Assuming Total Homogeneity in Composite (Eq X3.28)

m	*k*	*mk*	% Reduction
1	1	1	0
	2	2	29
	3	3	42
	4	4	50
	5	5	55
	10	10	68
2	1	2	29
	2	4	50
	3	6	59
	4	8	65
	5	10	68
	10	20	78
3	1	3	42
	2	6	59
	3	9	67
	4	12	71
	5	15	74
	10	30	82

(9) Classification Problem — Some discussions on classification are given in Principles of Environmental Sampling.[9]

(10) Let $x_1, \ldots, x_n$ be n individual samples and y_k ($k \leq n$) be a composite sample of k individual samples. Classification into two categories (for example, presence or absence of a contaminant) is to be made on each x based on analysis of y_k first, and perhaps some or all of the x's if y_k is positive.

(11) Because compositing may dilute the concentration to a level below detection limit, the number k can be determined to ensure that this does not happen.

(12) Assume that one individual sample has concentration C and all the other (k–1) samples have concentration zero. Then the composite concentration is:

$$y_k = C/k \tag{X3.31}$$

Given that the detection limit is d, we want a number k such that

$$C/k > d \tag{X3.32}$$

Namely,

$$k < C/d \tag{X3.33}$$

(13) If regulatory limit L is the concern, instead of d, then Eq X3.30 can be modified to to find the right k:

$$k < L/d \tag{X3.34}$$

(14) In the case of using Eq X3.34, if $y_k < L$, then $x_i < L$, i=1, . . ., k. Namely, it can be concluded that all the individual samples are less than the regulatory limit L. And only one analysis of the composite sample is required to reach this conclusion.

(15) If $y_k \geq L$, then the simplest scheme is to analyze all the individual samples to determine if any exceeds the limit. And the total number of analysis is (k+1).

(16) Let q = probability ($y_k < L$), then the expected number of analyses under compositing is:

$$E(N) = q + (1–q)\,(k+1) \tag{X3.35}$$

(17) Thus, the cost saving potential of composite sampling can be measured by the following relative efficiency index (REI), which is the ratio of the expected number of analyses under composite sampling to the number of analyses for individual samples:

$$\text{REI} = E(N)/k = 1 – q + 1/k = p + 1/k \tag{X3.36}$$

where:

p = $1 – q$
= probability of exceedance.

(18) Savings from compositing is realized when p is small and only when REI<1, which translates into:

$$\text{REI} < 1 \tag{X3.37}$$
$$1 – q + 1/k < 1$$
$$q > 1/k$$

Or,

$$0 < p < 1 – 1/k \tag{X3.38}$$

[9] Keith, L. H., *Principles of Environmental Sampling*, L. H. Keith, ed., American Chemical Society, 1988.

(19) The example percent reductions in the total number of analyses as a function of k and p in Eq X3.36 are given in Table X3.5.

TABLE X3.5 Relative Efficiency of Composite Sampling versus Individual Tests (Eq X3.36)

k	REI<1	p	REI	% Savings Relative to Individual Tests
2	p<0.50	0.4	0.9	10
		0.3	0.8	20
		0.2	0.7	30
		0.1	0.6	40
		0.05	0.55	45
		0.01	0.51	49
3	p<0.67	0.4	0.73	27
		0.3	0.63	37
		0.2	0.53	47
		0.1	0.43	59
		0.05	0.38	62
		0.01	0.34	66
4	p<0.75	0.4	0.65	35
		0.3	0.55	45
		0.2	0.45	55
		0.1	0.35	65
		0.05	0.30	70
		0.01	0.26	74
5	p<0.80	0.4	0.6	40
		0.3	0.5	50
		0.2	0.4	60
		0.1	0.3	70
		0.05	0.25	75
		0.01	0.21	79
10	p<0.90	0.4	0.5	50
		0.3	0.4	60
		0.2	0.3	70
		0.1	0.2	80
		0.05	0.15	85
		0.01	0.11	89