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Visual Sample Plan (VSP) Models and Code Verification

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Summary

Visual Sample Plan (VSP) is an easy-to-use visual and graphic software tool being developed to select the right number and location of environmental samples so that the results of statistical tests performed to provide input to environmental decisions have the required confidence and performance. It is a significant help in implementing Steps 6 and 7 of the Data Quality Objectives (DQO) planning process ("Specify Tolerable Limits on Decision Errors" and "Optimize the Design for Obtaining Data," respectively).

This report documents 1) the models (equations) in the VSP program that are used to compute the approximate number of samples needed for an environmental sampling study; 2) the activities conducted by Pacific Northwest National Laboratory (PNNL) to verify that those models are scientifically sound and correctly programmed and implemented in VSP; and 3) an evaluation of the nonstatistical user-interface aspect of the VSP program.

PNNL researchers performed this evaluation on Version 0.9H; needed corrections were incorporated into Version 0.9I.

This report first discusses

- the equations used in VSP to approximate the number of samples (sample size) needed for statistical tests of hypotheses
- the testing conducted previously to verify the accuracy of VSP calculations of the sample size needed to detect "hot spots" or of the probability of detecting "hot spots" for a specific number of samples
- the assumptions that underlie each sample-size equation
- the technical basis and scientific source (peer-reviewed scientific papers, books) of each sample-size equation
- the calculations conducted by hand and by an independent computer program, S-PLUS, to verify the accurateness of the sample-size computations in VSP
- possible alternative methods for determining the number of samples that may be of interest for future implementation within VSP.

The calculations of sample size conducted by hand as well as by S-PLUS confirmed that Version 0.9H of VSP was correctly and accurately computing sample sizes except for the one-sample test of proportion when the null hypothesis was stated as "the site is clean." The VSP code was modified to correct this error for Version 0.9I. Also, the method used in Version 0.9H for computing the two-sample test of proportions was changed in Version 0.9I to be consistent with the corrected method for the one-sample test of proportion. The only other significant problem identified was that, in some cases, Version 0.9H displayed an incorrectly drawn Decision Performance Goal Diagram (DPGD) for the MARSSIM sign test and the Wilcoxon rank sum test. This problem also was corrected in Version 0.9I.

In addition, this report discusses

- a series of steps to test the installation of VSP on various versions of the Windows operating system
- verification tests of the import, export, and removal of random sampling locations

- verification tests of five VSP drawing functions
- verification tests of the correspondence between values in selected VSP dialog boxes and the Report View, Graph View, Map View, and Coordinates View
- documentation of algorithms to determine sampling location by regular simple random sampling, adaptive-fill simple random sampling, and systematic grid sampling
- documentation of the two random number generators used in VSP
- the MATLAB code used to produced random test data
- the random test data used to check the correspondence of values in VSP dialog boxes and the Report View, Graph View, Map View, and Coordinates View.

With regard to these tests of Version 0.9I, all were conducted successfully. Occasional problems with regard to the input of certain values for the two-sample t-test option were found in Version 0.9H. Also, the DPGD graph subtitle for this option did not display the alpha and beta decision error rates. Both problems were corrected in Version 0.9I. Also corrected was a problem related to the removal of sampling locations by the use of a comma-delimited ASCII text file of coordinate locations. Other corrections were made for Version 0.9I: the Total Cost calculation was applied consistently to all options, and the DPGD graph for the Wilcoxon rank sum test was corrected for null hypothesis "Site is Clean."

Version 0.9I of VSP replaced Version 0.9H on the Internet on February 1, 2001. It is anticipated that Version 0.9I will be converted directly into Version 1.0 upon completion of documentation contained herein, the finalization of a users manual (under development), and external peer review conducted by the U.S. Environmental Protection Agency (EPA).

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Abbreviations and Acronyms

DQO   Data Quality Objectives

DPGD   Decision Performance Goal Diagram

DXF   Data Exchange Format

EPA   U.S. Environmental Protection Agency

GIS   geographic information system

GPS   global positioning system

MARSSIM   Multi-Agency Radiation Survey and Site Investigation Manual

MQO   Measurement Quality Objectives

PNNL   Pacific Northwest National Laboratory

VSP   Visual Sample Plan

WRS   Wilcoxon rank sum

1.0 Introduction

Visual Sample Plan (VSP) is a software tool under development at the Pacific Northwest National Laboratory (PNNL) for the U.S. Environmental Protection Agency (EPA). VSP will select the right number and location of environmental samples so that the results of statistical tests performed to provide input to environmental decisions have the required confidence and performance. Version 0.9H of VSP provides sample-size equations or algorithms needed by specific statistical tests appropriate for the following three environmental sampling scenarios:

- Comparing representative measurements from a defined geographical area to a fixed threshold (upper limit) value.
- Comparing representative measurements from one defined geographical area with representative measurements from another geographical area.
- Looking for areas of elevated concentration ("hot spots") at a study site.

This report presents the equations and underlying assumptions used to compute the sample sizes in Version 0.9H of VSP. It then documents the activities and quality checks conducted by PNNL

- to assess the technical and scientific basis of the sample-size equations used in Version 0.9H
- to verify that the sample-size equations are correctly programmed and implemented in the VSP computer code
- to evaluate the correctness of the nonstatistical elements of the user interface and input/output procedures.

The key features and capabilities of the VSP software tool are outlined and illustrated in Section 2. In Section 3, the statistical methods and computations underlying the program's sample-size equations are presented, followed by a description of how PNNL verified the scientific and technical soundness of the equations and the extent to which they are implemented correctly in the VSP program. PNNL's evaluation of the nonstatistical components of VSP is documented in Section 4.

2.0 Visual Sample Plan Program Overview

Visual Sample Plan (VSP) is easy to use and is highly visual and graphic. It is a significant help in implementing the sixth and seventh steps of the Data Quality Objectives (DQO) planning process ("Specify Tolerable Limits on Decision Errors" and "Optimize the Design for Obtaining Data," respectively). In particular, the program prompts the user to specify decision performance requirements by constructing the Decision Performance Goal Diagram (DPGD) discussed in EPA (2000a). VSP is designed primarily for project managers and users who are not statistical experts, although individuals with statistical expertise also will find the program useful. VSP is applicable to any two-dimensional geographical population to be sampled, including surface soil, a defined layer of subsurface soil, building surfaces, water bodies, or other similar applications. The VSP user can display graphical outputs in the "Quad Window" option, as shown in Figure 2.1.

After opening the VSP program, the user imports or constructs a visual map of the study site to be sampled. Only simple techniques are needed for map import or construction. The study site may be only a portion of a complex facility, the map of which has been imported into VSP (see Figure 2.1).
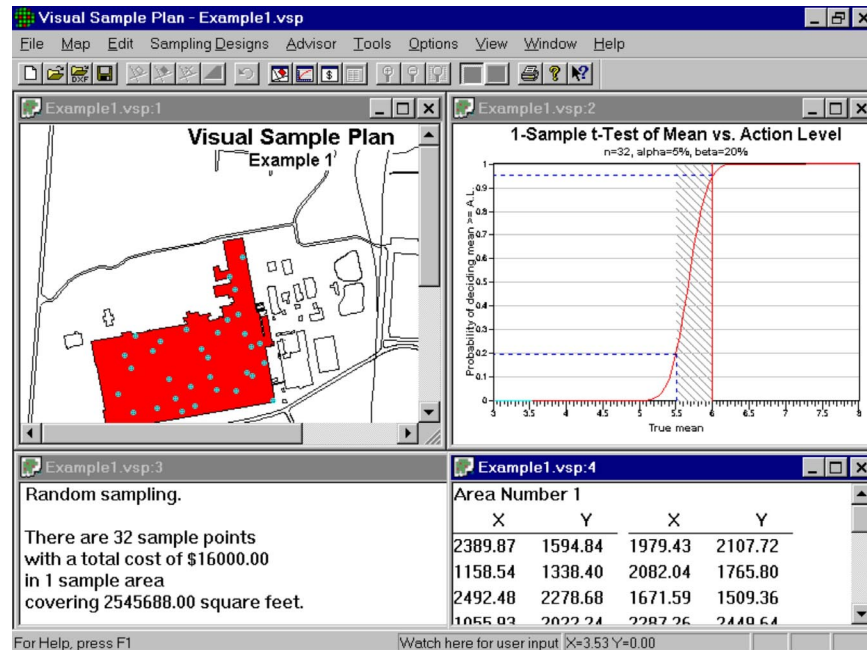
Figure 2.1. VSP Quad Window Display

Then, for the user-specified sampling objective, VSP leads the user through the quantitative steps of the DQO process (Steps 6 and 7) so that VSP has the information needed to compute the recommended minimum number of samples (sample size). Moreover, VSP contains a Measurements Quality Objectives (MQO) module that enables the user to assess the cost and benefits of two alternative analytical measurement protocols and permits an evaluation of the tradeoffs between taking more samples or performing replicate analyses on each sample.

The locations of the samples over the study site are determined by the specific sampling design (pattern) selected in VSP by the user. Version 0.9H of VSP permits the user to select simple random sampling, systematic sampling (using square, rectangular, or triangular spacing between locations), and judgment sampling. VSP provides two types of random number generators for randomly selecting a sampling location for the simple random sampling option: 1) a pseudo-random number generator, for which each potential location has an equal and independent chance of being selected, and 2) a quasi-random number generator (Press et al. 1992), for which locations are chosen to be somewhat more evenly spaced than would be obtained using the pseudo-random number generator. Version 0.9H also enables the user to add sample points to a current design either manually (subjectively) or using an automatic algorithm called Adaptive Fill. The Adaptive Fill algorithm adds data points in such a way as to avoid existing sampling locations.

VSP displays the sample locations determined by VSP on the site map for easy visualization (see Figure 1, upper left corner). VSP also lists the geographical coordinates of the sample locations (see Figure 1, lower right corner), which can be saved and exported as a Data Exchange Format (DXF) file for use in a geographical information system (GIS) or global positioning system (GPS) software.

VSP also displays the DPGD specified by the user for determining the number of samples (see Figure 1, upper right corner). The DPGD graphically shows the user-supplied acceptable probabilities of making decision errors based on the data obtained using the sampling design and number of samples. These probabilities are used by VSP to compute the number of samples needed. VSP also documents the selected sampling pattern (random, systematic, or judgment), the minimum number of samples computed by the program, and the total cost of sampling and measurements, as well as any relevant statements on the probability that the selected sampling design will detect "hot spots" (see Figure 1, lower left corner).

The user has the option of using the MQO module, which is operational for most of the statistical tests in Version 0.9H. The MQO module will compute the number of field samples required for a specified analytical method when the user specifies the number ($r = 1, 2,$ or 3) of replicate analyses being considered, the variability in the data due to only the analytical measurement process in the laboratory, and the variability due to sampling and all other sources of variability prior to the analytical measurement process. The user is asked to also specify the "overhead" costs (e.g., costs of planning and quality assurance), field collection cost per sample, and analytical measurement process cost per aliquot.

The user has the option of supplying analytical measurement process cost and variability information for an alternative type of analytical measurement process method that the VSP user has indicated is also available. In that case, VSP will compute the number of field samples and the total costs of the two sampling and analytical programs, both of which will achieve the performance requirements specified in the DPGD. This permits the user to select the most economical measurement method that achieves the DPGD goals (DQOs).

3.0 Verification and Documentation of Statistical Methods and Computations

The activities conducted in evaluating the statistical methods and computations contained within Version 0.9H of the VSP code are documented in this section.

To assess the scientific basis of the sample-size equations in VSP, PNNL used two criteria:

- Were the sample-size equations used published in peer-reviewed scientific publications?
- Did the EPA or other government or regulatory agency publications and guidance documents recommend the sample-size equations for environmental applications?

Although alternative methods are available for determining the number of samples, conducting the necessary computer simulation studies needed to demonstrate their advantages and disadvantages was beyond the scope of PNNL's project. The current methods in VSP are valid for the assumptions used in their mathematical derivation. These assumptions are documented for each statistical test discussed in Section 3.1. The user of Version 0.9H (and the updated Version 0.9I) of VSP must determine if the assumptions are reasonable for the site of interest and seek help from a statistical expert if assumptions are seriously violated.

To verify that the equations were programmed correctly, the number of samples computed using the sample-size equations in VSP were compared with hand calculations as well as those obtained by an independent exercise of the equations using a constructed S-PLUS $^{(R)}$ computer code. This verification activity is discussed in Section 3.2.1.

The correctness of the VSP calculations for determining the number of samples needed to detect hot spots was checked, as discussed in Section 3.2.2. Also, the correctness of the DPGDs and all other outputs provided by VSP for each sample-size equation were checked, as discussed in Section 3.2.3.

3.1 Technical Basis of Sample-Size Equations in VSP

Each of the following subsections corresponds to one of the three sampling scenarios listed in Section 1.0. Within each subsection, PNNL's findings regarding the VSP sample-size equations or methods used to obtain the sample size are provided, along with scientific references that document their derivation and use. The notation used in the equations is defined in Table 3.1.

For the MQO modules, we assume a two-component additive variance model such that the total random statistical variance can be expressed as the sum of the sampling variance and the analytical variance. In reality, there are many components of error/uncertainty that affect both the sampling and analytical variance. Our intent in VSP is to define any random variations that could occur due to activities outside the analytical laboratory as sampling variations, estimated as s^2_{sample}, and any random

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$^{(R)}$ S-PLUS is a registered trademark of the Insightful Corporation, Seattle, Washington.

variations that could occur within the analytical laboratory as analytical variance , estimated as $s^2_{analytical}$.

Sampling variations could include variations due to spatial differences, sample handling, field sampling methods and instruments, or field activities or other similar activities occurring outside the analytical laboratory. Analytical variations are variations that can be observed among r different portions of the field sample that undergo separate analytical treatment in the laboratory. Thus analytical variations, $s^2_{analytical}$, may include variations due to sample preparation, dilution, fusion, sample splitting, calibration, measurement, or instrument variations or similar variations that are associated with the analytical laboratory. In VSP, it is assumed that the entire analytical process in the laboratory, from sample aliquoting and preparation through instrument measurements, is repeated for each of the r portions of the field sample. The VSP MQO options are applicable to any two-component variance model as long as the definitions of the r different portions of the field sample and the estimated analytical variance ($s^2_{analytical}$) are consistent with that variance model. The VSP MQO options can be used when the estimated analytical variance ($s^2_{analytical}$) supplied by the VSP user includes only those parts of the total variance that are added during the analytical process applied to each of the r portions of the field sample.

Table 3.1. Some Common Notation Used in VSP Sample-Size Equations

Notation	Description
n	the minimum recommended number of samples that should be collected from a site, as computed using one of the sample-size equations in VSP
r	the number of measurements (analytical replicates) that will be obtained for each field sample
α	the probability that the VSP user specifies willingness to tolerate that a Type I decision error will be made, i.e., that the data collected and used in the appropriate statistical test will falsely reject the null hypothesis. For example, if the null hypothesis is "the mean concentration at the site *exceeds* the action limit," then α is the probability the VSP user can tolerate that the statistical test computed using the n data will incorrectly indicate that the mean concentration does not exceed the action limit, in short, calling a dirty site clean.
β	the probability the VSP user specifies willingness to tolerate that a Type II decision error will be made, i.e., that the data collected and used in the appropriate statistical test will falsely accept the null hypothesis. For example, if the null hypothesis is that the mean concentration at the site exceeds the action limit, then β is the probability the VSP user can tolerate that the statistical test computed using the n data will falsely indicate the mean concentration does exceed the action limit, in short, calling a clean site dirty.

Table 3.1. Common Notation (contd.)

Notation	Description
Δ	the width of the "gray region" in the Decision Performance Goal Diagram (DPGD) used in the DQO process (EPA 1994) and in VSP. For example, if the sampling objective is to compare the true mean of the site to the true mean of a background area, then Δ is the difference between the true site mean and the true background mean that the VSP user specifies is important to detect with (high) probability $1 - \beta$. Similarly, if the objective is to compare the mean of the site to a fixed action limit, then Δ is the difference between the true mean and the action limit that is important to detect with (high) probability $1 - \beta$.
σ^2_{total}	the true "total variance" of the population of all possible measurements made on all possible samples collected from the study site. The model of the true total variance used in Version 0.9H of VSP is $\sigma^2_{total} = \sigma^2_{sample} + \sigma^2_{analytical}$, where $\sigma^2_{analytical}$ is the true variance component due to the analytical measurement process in the laboratory and σ^2_{sample} is the true variance component due to all other sources of variation, including variations in true concentrations at different study site locations and the variance added due to selecting, collecting, and transporting samples to the laboratory.
s^2_{total}	the computed *estimate* of the true total variance, σ^2_{total}. If r = 1 for all n field samples, then the quantity s^2_{total} is computed as $$s^2_{total} = \frac{\sum_{i=1}^{n}(x_i - \bar{x})^2}{n-1},$$ where x_i is the measurement obtained for a single aliquot extracted from the ith field sample and $\bar{x}$ is the arithmetic mean of the n representative measurements, x_i.
s^2_{sample}	an estimate of the total variance of the data x_i that would be obtained if $\sigma^2_{analytical} = 0$
$s^2_{analytical}$	an estimate of the total variance of the data x_i that would be obtained if the only variability in the data were due to the analytical process, i.e., if $s^2_{sample} = 0$
$t_{1-\alpha,df}$	the value of the Student's t-distribution with df <u>d</u>egrees of <u>f</u>reedom. By definition, the proportion of the distribution to the left of the value $t_{1-\alpha,df}$ is $1-\alpha$. A table of the values of $t_{1-\alpha,df}$ is found in most statistics books, e.g., Gilbert (1987, Table A2).

Table 3.1. Common Notation (contd.)

Notation	Description
$Z_{1-\alpha}$	the value from the standard normal distribution for which the proportion of the distribution to the left of $Z_{1-\alpha}$ is 1-α. A table of the values of $Z_{1-\alpha}$ is found in most statistics books, e.g., Gilbert (1987, Table A1). If the selected probability of a false rejection, α, is made smaller, then 1- α will be larger and $Z_{1-\alpha}$ will be larger, leading to larger sample sizes. If the null hypothesis is that concentrations at the site *exceed* the action limit, i.e., that the site is "dirty," then $Z_{1-\alpha}$ can be thought of as an index number whose magnitude quantifies the strength of our desire to avoid deciding a dirty site is clean.
$Z_{1-\beta}$	the value of the standard normal distribution for which the proportion of the distribution to the left of $Z_{1-\beta}$ is 1-β. If the selected probability of a false acceptance, β, is made smaller, then 1-β and $Z_{1-\beta}$ will be larger, leading to larger sample sizes. If the null hypothesis is that concentrations at the site *exceed* the action limit, i.e., that the site is "dirty," then $Z_{1-\beta}$ can be thought of as an index number whose magnitude quantifies the strength of our desire to avoid deciding a clean site is dirty.
$\Phi(z)$	the cumulative standard normal distribution function, i.e., $$\Phi(z) = \tfrac{1}{\sqrt{2\pi}} \int_{-\infty}^{z} e^{-\frac{1}{2}x^2} dx .$$ A table of $\Phi(z)$ values is provided in most statistics books, e.g., Gilbert (1987, Table A1).

3.1.1 Comparing a Population to a Fixed Upper Limit

Suppose a VSP user wants to determine the number of samples, n, that should be collected in order to decide if the true average concentration exceeds a specified risk-based or regulatory-based upper limit. For this situation, VSP provides several different equations for computing the number of samples, n, given that the VSP user has specified the number of analytical replicates, r, that will be made for each field sample.

The equation selected for computing the number of samples to decide if the true average exceeds the fixed standard depends on whether the VSP user is going to use the measurements in a "one-sample" t- test, a Wilcoxon signed ranks test, the one-sample test for proportions, the Sign test (the "MARSSIM Sign test"), or will compute a confidence interval for the mean. The sample-size equation for each test is provided below, along with the assumptions that underlie the use of that test. An assumption common to all tests is that the measurements at different locations are not correlated.

One-Sample t-Test

The one-sample t-test can be used to test if the true mean of the study-site population of interest exceeds a fixed upper limit. The equation used in VSP to compute the minimum recommended number

of samples, n, needed for the test when the VSP user specifies that only r = 1 analytical replicate from each sample will be made is

$$n = \frac{s_{total}^2 (Z_{1-\alpha} + Z_{1-\beta})^2}{\Delta^2} + 0.5 Z_{1-\alpha}^2$$

(3.1)

However, if the MQO module in VSP is used, in which case r = 1, 2, or 3 analytical replicates of each field sample can be made, then the equation used in VSP to compute n is

$$n = \frac{\left(s_{sample}^2 + \dfrac{s_{analytical}^2}{r}\right)(Z_{1-\alpha} + Z_{1-\beta})^2}{\Delta^2} + 0.5 Z_{1-\alpha}^2$$

(3.2)

The notation used in Equations (3.1) and (3.2) is defined in Table 3.1. These equations are computed using the values of α, β, Δ, r, s_{total}, s_{sample}, and $s_{analytical}$ that are specified by the VSP user.

The assumptions that underlie the derivation of Equation (3.1) are that the data are normally distributed and representative of the study site and are not spatially or temporally correlated, and that $\bar{x} - ks_{total}$ is normally distributed with mean $\mu - k\sigma$ and variance $(\frac{\sigma^2}{n})(1 + \frac{k^2}{2})$, where k is a given constant (Guenther 1981). The derivation of Equation (3.1) is found in Wallis (1947), Guenther (1977), EPA (2000a, Appendix A) and EPA (1992, pp. F-8, F-9, and F-10). Equation (3.1) is used in the statistics book by Bowen and Bennett (1988, pp. 155, 156) and in EPA (2000a), EPA (1994b, p. 21), and EPA (2000b, pp. 3-7).

Guenther (1981) indicates that although Equation (3.1) is an approximation to the true minimum sample size required for the one-sample t-test, Equation (3.1) usually yields the exact solution for n. The exact solution is obtained using an iterative approach using tables of the non-central t distribution found in Owen (1965).

Equation (3.2) also should provide a very accurate approximation of n for a specified r value because it is a straightforward extension of Equation (3.1) to the case of r > 1 analytical replicates for each field sample. For this case, it is easily shown that the total variance is estimated by computing

$$s_{total}^2 = s_{sample}^2 + \frac{s_{analytical}^2}{r}$$

If this equation for s_{total}^2 is inserted in Equation (3.1), then Equation (3.2) is obtained.

Methods other than Equations (3.1) and (3.2) have been proposed also for approximating n for the one-sample t-test. For example, Desu and Raghavarao (1990, p. 10) give a two-stage t-test procedure. Also, a PNNL statistician who peer-reviewed VSP for this project suggests that an iterative approach using the t distribution to determine n should be considered when n computed using Equation (3.1) is small (see the first comment in Appendix A). However, these alternative methods for determining n, as well as the exact method mentioned above, have not been studied and compared with Equations (3.1) and (3.2). A computer simulation study to examine this issue is being considered as part of the future development of VSP.

Wilcoxon Signed Ranks Test

The Wilcoxon signed ranks test can be used to test whether the true median or mean of the study-site population exceeds a fixed upper limit. The assumptions needed for this test are that the data are representative of the study site, are not spatially or temporally correlated, and have a symmetric (but not necessarily normal) distribution. Note that the test applies to either the mean or median because those two population parameters are identical when the population of measurements has a symmetric distribution.

The equation used in VSP to compute a lower bound on the number of samples, n, needed for the test when the VSP user specifies that only $r = 1$ analytical replicates from each field sample will be obtained is

$$n = 1.16\left[\frac{s_{total}^2\left(Z_{1-\alpha} + Z_{1-\beta}\right)^2}{\Delta^2} + 0.5Z_{1-\alpha}^2\right] , \tag{3.3}$$

which is used in *Guidance for Data Quality Assessment* (EPA 2000b, pp. 3-12).

If the MQO module for this test is used, in which case $r = 1, 2,$ or 3 can be used, then the equation for n used in VSP is

$$n = 1.16\left[\frac{\left(s_{sample}^2 + \dfrac{s_{analytical}^2}{r}\right)\left(Z_{1-\alpha} + Z_{1-\beta}\right)^2}{\Delta^2} + 0.5Z_{1-\alpha}^2\right] \tag{3.4}$$

Note that Equation (3.3) is identical to Equation (3.1) and Equation (3.4) is identical to Equation (3.2) except for the 1.16 multiplier. Hence, n computed by VSP for the Wilcoxon signed ranks test is always 1.16 times larger than the n computed for the one-sample t-test using Equation (3.1). The constant 1.16 is used because it is known (see, e.g., Conover 1980, p. 291) that the Wilcoxon signed rank test will require no more than 1.16 times as many samples as the t-test to achieve the α and β decision error rate test performance specifications provided by the VSP user if the two symmetric population distributions are identical except for a difference in means.

Noether (1987, Section 2.2) developed an alternative to Equation (3.3) for computing n needed for the Wilcoxon signed ranks test. His method does not require that the data have a symmetric distribution. The assumptions that underlie his method are that the data are representative of the underlying population, the data are not correlated, and the computed Wilcoxon signed ranks test statistic (the quantity computed using the data to make the test) is approximately normally distributed. Noether (1987) indicates that the value of n computed using his method should achieve the performance requirements for the test (as specified by α and β) unless the computed n is "quite small."

The authors of this report are not aware of any studies that assess how well values of n computed using Noether's method result in the attainment of α and β test performance requirements. PNNL researchers are considering a computer simulation study to examine whether Equation (3.3) or Noether's equation should be used in VSP. Also, further study may be necessary to develop a Noether-type equation that would be used in place of Equation (3.4) when more than one analysis per sample is desired.

One-Sample Test for Proportions

The one-sample test for proportions which is discussed in EPA (2000b, pp. 3-18, 3-19, 3-20), evaluates whether the true proportion of the population of measurements that exceeds some concentration limit is greater than a specified fixed (standard) proportion. The assumptions needed for the test are that the data are representative and noncorrelated. The test is valid regardless of the shape of the data distribution. Hence, the data need not be normally distributed.

The equation used in VSP to compute the approximate number of samples required for the test when the VSP user specifies that only r = 1 analytical replicate of each field sample will be measured is

$$n = \frac{\left[Z_{1-\alpha}\sqrt{P_0(1-P_0)} + Z_{1-\beta}\sqrt{P_1(1-P_1)}\right]^2}{(P_1 - P_0)^2} \qquad (3.5)$$

where P_0 is the fixed (standard) proportion and P_1 is a specified value of the proportion different from P_0 that the VSP user indicates is important for the test to detect with probability $1-\beta$. VSP asks the user to specify P_0 and Δ, where Δ is the absolute value of P_1 - P_0, i.e., the positive difference between P_1 and P_0 (the width of the "gray region"). Once P_0 and Δ are specified, then VSP computes P_1. VSP computes P_1 as $P_1 = P_0 - \Delta$ if the VSP user specifies the null hypothesis to be "site does not meet the standard," whereas VSP computes P_1 as $P_1 = P_0 + \Delta$ if the null hypothesis is "the site meets the standard." This difference in the way P_1 is computed can result in different sample sizes, depending on the null hypothesis selected.

No MQO module is provided in Version 0.9H of VSP for the one-sample test of proportions. Hence, no equations analogous to Equations (3.2) and (3.4) are available for this test.

Equation (3.5) is derived in Bowen and Bennett (1988, p. 190) and used in EPA (2000b, p. 3-19), EPA (1992, p. 5-40), and EPA (1989, p. 7-6). Desu and Raghavarao (1990, p. 16) compute n using a more complicated approximate formula. Equation (3.5) was used in VSP because it is simpler, easier to understand, and is used in EPA guidance documents. We are not aware of any study that indicates the method in Desu and Raghavarao (1990) is more accurate. Computer simulations to make this evaluation are being considered as part of the further development of VSP.

Sign Test (MARSSIM Sign Test)

The sign test can be used to test whether the true median concentration of the population being sampled exceeds a fixed upper limit value. The formula used to compute the approximate number of samples, n, needed for the sign test when only r = 1 analytical replicates per field sample will be obtained is given in the Multi-Agency Radiation Survey and Site Investigation Manual (MARSSIM) (EPA 1997, p. 5-33):

$$n = 1.20\left[\frac{\left(Z_{1-\alpha} + Z_{1-\beta}\right)^2}{4\left(SignP - 0.50\right)^2}\right] \tag{3.6}$$

where

$$SignP = \Phi\left(\frac{\Delta}{s_{total}}\right) \tag{3.7}$$

Equation (3.7) is derived in Gogolak, Powers, and Huffert (1997, pp. 9-3 and 9-7).

VSP denotes the sign test as the MARSSIM sign test to signify that Equation (3.6) is taken from the MARSSIM document (EPA 1997). The function Φ (defined in Table 3.1) denotes the cumulative distribution function of the standard normal distribution (a normal distribution with mean zero and standard deviation 1). Hence, by definition, $\Phi\left(\frac{\Delta}{s_{total}}\right)$ is the fraction of the bell-shaped standard normal distribution that is less than or equal to the value of $\frac{\Delta}{s_{total}}$. Note that $\frac{\Delta}{s_{total}} > 0$ because Δ, the width of the gray region in the DPGD, must be greater than zero. VSP computes Sign P = $\Phi\left(\frac{\Delta}{s_{total}}\right)$ using the value of $\frac{\Delta}{s_{total}}$ specified by the VSP user. We note that the MARSSIM document (EPA 1997, Table 5.4, p. 5-32) provides values of Sign P for some values of $\frac{\Delta}{s_{total}}$ between 0.1 and 3.0.

If the VSP user makes use of the MQO module, in which case r = 1, 2, or 3 analytical replicates per field sample will be obtained, then

3.8

$$SignP = \Phi \left[\frac{\Delta}{\left(s^2_{sample} + \frac{s^2_{analytical}}{r} \right)^{1/2}} \right] \qquad (3.8)$$

Equation (3.6) is based on the formula for n proposed by Noether (1987, Section 2.1) for the sign test. His equation for n is identical to Equation (3.6) except that Noether used the constant 1.00 in place of 1.20. The assumptions that underlie Noether's equation are that the data are representative of the underlying population, the data are not correlated, and the computed sign test statistic (the quantity computed using the data to make the test) is approximately normally distributed.

Noether (1987) indicates that the value of n computed using his method should achieve the performance requirements for the sign test (as specified by α, β, and Δ) unless the computed n is "quite small." The MARSSIM report (EPA 1997) used 1.20 instead of 1.00 in Equation (3.6) to provide subjective added confidence that the larger value of n computed would result in achieving the performance requirements specified for the test by the VSP user.

Equation (3.6) is used in VSP primarily because it is used in EPA (1997), which is a multi-agency consensus document that was developed collaboratively by four federal agencies having authority and control over radioactive materials: the U.S. Departments of Defense and Energy, the U.S. Nuclear Regulatory Commission, and the EPA.

Confidence Interval for the Mean

Rather than use one of the tests above, one could assess whether the true mean exceeds the action level by computing a one-sided or a two-sided confidence interval for the mean and looking to see if that interval overlaps the limit. For that case, one needs to determine the number of samples required to compute the confidence interval.

The equation used in VSP to compute the minimum recommended value of n for a one-sided confidence interval when only r = 1 analytical replicates per field sample is

$$n = \left(\frac{t_{1-\alpha,df}}{d} \right)^2 s^2_{total} \qquad (3.9)$$

where d denotes the VSP user's largest acceptable difference between the estimated mean, $\bar{x}$, and the true mean μ. In other words, the VSP user specifies that n should be large enough such that the absolute value of $\bar{x}$ - μ will be no larger than the specified value of d with 100 (1- α) percent confidence. The quantity d can be interpreted also as the width of the one-sided confidence interval on μ that the VSP user specifies should not be exceeded. If a two-sided confidence interval is used, then d is the *half*-width of that interval.

3.9

The notation $t_{1-\alpha,df}$ and s^2_{total} are defined in Table 3.1, where df = degrees of freedom = n-1. Thus, n appears on both sides of Equation (3.9). Hence, Equation (3.9) is solved iteratively in VSP to determine the smallest n that satisfies the equality sign. The iteration scheme used is in Gilbert (1987, p. 32). Equation (3.9) is a standard formula found in many statistics books, e.g., Hahn and Meeker (1991, p. 136), Iman and Conover (1983, p. 188), and Gilbert (1987, p. 32).

If the MQO module is used, in which case r = 1, 2, or 3 analytical replicates per field sample can be specified by the VSP user, then

$$n = \left(\frac{t_{1-\alpha,df}}{d}\right)^2 \left(s^2_{sample} + \frac{s^2_{analytical}}{r}\right) \tag{3.10}$$

Equation (3.10) is a straightforward extension of Equation (3.9).

If the VSP user wants to use a two-sided confidence interval to test whether the true mean exceeds the action limit, then $t_{1-\alpha,df}$ in Equation (3.9) and Equation (3.10) is replaced by $t_{1-\alpha/2,df}$. Furthermore, d is now the half-width of the confidence interval that must be achieved.

Hahn and Meeker (1991, pp. 137-141) suggest two alternative methods for computing n. It is beyond the scope of the work reported here to evaluate whether these alternative methods are more accurate than Equations (3.9) and (3.10).

3.1.2 Comparing Two Populations

Suppose a VSP user wants to determine the number of samples, n, that should be collected at a study site and also the number of samples, m, that should be collected in a reference site (e.g., a background area) to decide if the true average site concentration exceeds the true average reference area concentration. For this situation, VSP provides several different equations for computing the recommended minimum number of samples, n and m needed, with the restriction that n = m.

The equation selected for computing the number of field samples depends on whether the VSP user is going to use the measurements in a "two-sample" t-test, a Wilcoxon rank sum test, the MARSSIM Wilcoxon rank sum (WRS) test, or the two-sample proportion test. The equations used in VSP to compute n and m are provided in the following paragraphs along with the assumptions that underlie the use of the tests. An assumption common to all tests is that the measurements at different locations are not correlated.

Two-Sample t-test

The two-sample t-test is a standard statistical test that can be used to test if the true site mean exceeds the true reference-area mean. The assumptions underlying the test are that the data are normally distributed, uncorrelated, and representative of the underlying site and reference populations, and the variance of the site data equals the variance of the reference area data.

The equation used in VSP to compute the minimum recommended number of samples n and m to obtain from the study site and the reference area, respectively, when the VSP user specifies that only r = 1 analytical replicates per field sample will be made is

$$n = m = \frac{2s_{total}^2 \left(Z_{1-\alpha} + Z_{1-\beta}\right)^2}{\Delta^2} + 0.25Z_{1-\alpha}^2 \qquad (3.11)$$

However, if the MQO module in VSP is used, in which case r = 1, 2, or 3 analytical replicates at the site and reference-area can be specified by the VSP user, then the equation used in VSP to compute n and m is

$$n = m = \frac{2\left(s_{sample}^2 + \dfrac{s_{analytical}^2}{r}\right)\left(Z_{1-\alpha} + Z_{1-\beta}\right)^2}{\Delta^2} + 0.25\,Z_{1-\alpha}^2 \qquad (3.12)$$

The key assumption that underlies the derivation of Equation (3.11), in addition to the assumptions given above, is that

$$\bar{x}_{site} - \bar{x}_{reference} - 2k\left(\frac{s_{site}^2 + s_{reference}^2}{2}\right)^{1/2} \qquad (3.13)$$

is normally distributed with mean $\mu_{site} - \mu_{reference} - 2k\sigma$ and variance $(\frac{\sigma^2}{n})(2 + k^2)$, where k is an arbitrary constant (Guenther 1981).

The derivation of Equation (3.11) is found in a more general context in Guenther (1977), where the problem Guenther considers includes the two-sample t-test. Equation (3.11) is used in the statistics book by Bowen and Bennett (1988, p. 168) and in EPA (2000, p. 3-24).

Guenther (1981) indicates that Equation (3.11) is an approximation to the true minimum sample sizes n and m required for the two-sample t-test. However, he states that Equation (3.11) usually yields the exact solution for n and m. The exact solution is obtained using an iterative approach using tables of the non-central t distribution found in Owen (1965).

Equation (3.12) should provide a very accurate approximation of n and m for a specified r value because it is a straightforward extension of Equation (3.11) to the case of r $\geq$ 1.

Methods other than Equations (3.11) and (3.12) also have been proposed for approximating n and m for the two-sample t-test. Desu and Raghavarao (1990, pp. 31-33) give an iterative procedure as well as a two-stage procedure that use the t distribution. As part of future work, these alternative methods for determining n and m, as well as the exact method mentioned above, could be studied using computer simulations and the results compared with those obtained using Equations (3.11) and (3.12).

Wilcoxon Rank Sum Test

The Wilcoxon rank sum (WRS) test can be used to test whether the true median concentration at the study site is larger than the true median at the reference area. The assumptions that underlie the WRS test are that the site and reference data are representative of the site and reference areas, respectively, the data are not correlated, and the two population distributions are identical in shape and have the same variance. The two distributions need not be symmetric or normally distributed.

The equation used in VSP to compute the number of samples, n and m, for the site and reference areas is

$$n = m = 1.16 \left[\frac{2s_{total}^2 \left(Z_{1-\alpha} + Z_{1-\beta} \right)^2}{\Delta^2} + 0.25 Z_{1-\alpha}^2 \right] \tag{3.14}$$

Equation (3.14) is used in VSP primarily because it is used in EPA (2000b, p. 3-34). The constant 1.16 in Equation (3.14) is used because it is known (see, e.g., Conover, 1980, p. 226) that the WRS test will require no more than 1.16 times as many samples as the two-sample t-test to achieve the α and β test performance specifications provided by the VSP user if the two population distributions (site and reference area) are identical except for their true median values.

If the MQO module for the WRS test is used and r = 1, 2, or 3 analytical replicates per field sample is specified by the VSP user, then the equation for n and m used in VSP is

$$n = m = 1.16 \left[\frac{2 \left(s_{sample}^2 + \frac{s_{analytical}^2}{r} \right) \left(Z_{1-\alpha} + Z_{1-\beta} \right)^2}{\Delta^2} + 0.25 Z_{1-\alpha}^2 \right] \tag{3.15}$$

Note that Equation (3.14) is identical to Equation (3.11) and Equation (3.15) is identical to Equation (3.12) except for the 1.16 multiplier.

MARSSIM Wilcoxon Rank Sum (WRS) Test

Noether (1987, Section 3.0) developed an alternative equation for approximating the number of samples required for the WRS test. Noether's equation is

$$n + m = \frac{\left(Z_{1-\alpha} + Z_{1-\beta} \right)^2}{3 \left(P_r - 0.5 \right)^2} \tag{3.16}$$

where n + m is the sum of the minimum number of study-site and reference-area samples VSP recommends be used for the WRS test, assuming n = m. Noether (1987) assumed when deriving Equation (3.16) that the WRS test statistic was approximately normally distributed, although the data

themselves need not be normally distributed. Equation (3.16) is a special case of a more general equation given by Noether (1987, Section 3.0) that allows the number of samples from the site and reference area to be unequal.

Equation (3.16) is used in EPA (1987, p. 5-28, Equation 5-1) and in EPA (1992, p. 6.3). If the VSP user selects the MARSSIM WRS test option in VSP, Equation (3.16) will be computed. It should be noted that EPA (1992) uses the more general sample-size equation that allows for unequal numbers of samples in the two populations; it also includes an upward adjustment in n to take into account the expected rate of missing or unusable data.

The parameter P_r in Equation (3.16), the value of which must be specified by the VSP user, is the probability that a measurement of a sample collected at a random location at the study site is greater than a measurement of a sample collected at a random location in the reference area. The allowable values of P_r that can be specified are between 0.5 and 1.0. The difference P_r - 0.5 is a measure of the difference between the site and reference distributions the VSP user wishes to detect with high probability $1 - \beta$.

P_r is computed in VSP using

$$P_r = \Phi\left(\frac{\Delta}{\sqrt{2}\sigma_{total}} \right) \tag{3.17}$$

when only r = 1 analytical replicate per field sample is made. When the MQO module is used, in which case r = 1, 2, or 3 is specified, the following equation is used:

$$P_r = \Phi\left(\frac{\Delta}{\sqrt{2}\sqrt{s^2_{sample} + \dfrac{s^2_{analystical}}{r}}} \right) \tag{3.18}$$

Equations (3.17) and (3.18) assume the data are normally distributed because the function Φ is the cumulative normal distribution function (see Table 3.1.). Hence, although the WRS test itself does not require that the data be normally distributed, the assumption of normality is used to determine the number of samples needed. In addition, the validity of Equation (3.16) requires that the WRS test statistic is itself approximately normally distributed.

According to one PNNL reviewer,

"The sample size formula for the WRS test is suspect to me. It assumes the asymptotic normality of the test statistic. For small sample sizes this could give spurious results. I would like to see some simulations run to support the use of this sample size formula for both large and small sample sizes." (Appendix A, p. A.1).

To address these concerns and provide information needed to develop future versions of VSP beyond the current Version 0.9I, PNNL is considering conducting simulations to evaluate if Equation (3.16) provides sufficiently accurate estimates of n.

Two-Sample Test for Proportions

The two-sample test for proportions, which is discussed in EPA (2000b, pp. 3-28, 3-29 and 3-30), evaluates whether the proportion of the site population that exceeds some concentration limit is greater than the proportion of the reference area population that exceeds that limit. The assumptions underlying this test are that the data are uncorrelated and representative of the populations. The data need not be normally distributed.

The equation used in Version 0.9H of VSP, as well as in EPA (2000b, p. 3-29), to compute the approximate number of samples required for this test when the VSP user specifies r = 1 is

$$n = \frac{2(Z_{1-\alpha} + Z_{1-\beta})^2 \, \overline{P}(1 - \overline{P})}{(P_1 - P_2)^2} \tag{3.19}$$

where

P_2 = the estimated proportion in the reference area greater than the limit (entered by the user)

P_1 = the unknown proportion at the study site greater than the limit

$\overline{P} = (P_1 + P_2)/2$.

Version 0.9H of VSP determines the value of P_1 as follows:

$$P_1 = P_2 \pm \Delta$$

where

Δ = the minimum difference in proportions P_1 and P_2 to be detected with power $1 - \beta$ with $100(1 - \alpha)$ percent confidence

and P_1 is chosen so that $\overline{P}$ is closest to 0.5 in order to maximize the value of n computed using Equation (3.19). The above approach for specifying P_1 and P_2 requires that the user enter P_1 and Δ to determine n. However, P_1 and P_2 also could be estimated using data obtained from previous studies at the study site and reference area.

During the checking of Equation (3.19), it was discovered that $(P_1 - P_2)^2$ in the denominator of that equation was incorrect and should be replaced by $(\delta_0 - \delta_1)^2$, where

- δ_0 is a specified *difference* in proportions that defines the Action Level where the decision error rate α is specified
- δ_1 is a user-selected *difference* in proportions that defines the outer bound of the gray region where the decision error rate β is specified.

This correction to Equation (3.19) was made in Version 0.9I of VSP.

Alternative methods for approximating n are available in the statistical literature. For example, Bowen and Bennett (1988, p. 193, Equation 4.98) provide a slightly different version of Equation (3.19). Consideration is being given to providing one or two additional equations for computing n in future versions of VSP and for allowing the VSP user to enter values for both P_1 and P_2.

3.1.3 Looking for Areas of Elevated Concentrations ("Hot Spots")

Suppose a VSP user wants to determine the spacing of sampling locations at a study site that should be used to detect a hot spot of specified size. The VSP user can specify that the sampling locations should be laid out over the study area in a square, rectangular, or triangular pattern. VSP determines the optimum spacing between sampling locations using an implementation of a computer program called ELIPGRID-PC (Davidson 1995b). The events that led to the development of this program are now briefly summarized.

Singer and Wickman (1969) published an algorithm for calculating the probability of locating elliptical hot spots when sampling is done on a square, rectangular, or triangular grid pattern over space. Singer (1972) published a FORTRAN IV computer program, ELIPGRID, to automate the hot spot probability calculations. He also evaluated the efficiency of square and triangular grids in the search for elliptically-shaped hot spots (Singer 1975). Zirschky and Gilbert (1984) developed nomographs for answering the same questions addressed by ELIPGRID. These nomographs were published in Gilbert (1987, Chapter 10) along with examples of the calculations. Davidson (1995b) wrote and published ELIPGRID-PC for the personal computer, an upgraded and corrected version of the original ELIPGRID algorithm. ELIPGRID-PC was subsequently incorporated into VSP.

The assumptions that underlie the ELIPGRID-PC and the VSP implementation of that code are, from Gilbert (1987, pp. 119-120):

- The target (hot spot) is circular or elliptical. For subsurface targets, this assumption applies to the projection of the target to the ground surface.
- Samples or measurements are taken on a square, rectangular, or triangular pattern.
- The distance between grid points is much larger than the area sampled, measured, or cored at grid points; that is, a very small proportion of the area being studied can actually be measured.
- The definition of "hot spot" is clear and unambiguous; the types of measurement and the levels of contamination that constitute a hot spot are clearly defined.
- There are no measurement misclassification errors; that is, no errors are made in deciding when a hot spot has been found.

The computations conducted by VSP to determine the spacing of sampling locations are described in Singer (1972) and Davidson (1995b).

3.15

3.2 Verification of VSP Computations and Outputs

The activities conducted to verify that VSP is computing, displaying, and describing VSP outputs correctly and accurately are documented in this section. Section 3.2.1 presents the verification results for the simple random sampling option in VSP. These verification results also apply to the systematic sampling option in VSP because the equations used for that option are identical to those used for simple random sampling. Section 3.2.2 discusses verification results for the hot-spot detection option. The results of these verifications are summarized here and discussed fully in Davidson (2001).

It should be noted that the following three features of VSP were not verified by Davidson (2001) or as part of the scope of work for this project:

- the hot spot options that use numerical search algorithms
- the adaptive-fill sampling option
- the quasi-random sampling option.

3.2.1 Simple Random Sampling and Systematic Sampling

The accuracy of VSP computations of sample sizes when the simple random sampling or systematic sampling option is used was verified by comparing VSP sample sizes with those computed by hand and by a specially prepared computer test program, S-PLUS, written in the S language.

Comparisons of Sample Sizes Computed by VSP and S-PLUS When MQO Module Is Not Used

The sample sizes computed by both VSP and S-PLUS were compared for all the statistical tests described in Section 3.1 for the case of $r = 1$ analytical replicates per field sample (Davidson 2001). The null hypothesis used was "the site is dirty." For this $r = 1$ case, 15 test cases for each of the statistical tests were computer-generated. For each test case, a value of each parameter in the sample-size equation was generated from a uniform distribution. This process yielded 15 cases for each test that had a wide variety of parameter value combinations. Then the sample size for each test case was computed using both the VSP program and the S-PLUS program.

All VSP-calculated sample-sizes agreed with the sample sizes calculated by the S-PLUS program. The results for the one-sample t-test (Equation 3.1) are given in Table 3.2. The complete results for all statistical tests for the VSP and S-PLUS codes are provided in Davidson (2001). The S-PLUS test file and underlying computer code are given in Appendixes A and B, respectively, of Davidson (2001).

Table 3.2. Tests of VSP Code for Computing the Sample Size for the One-Sample t-test

Test Case	Alpha	Beta	Delta	Standard Deviation	Calculated Sample Sizes	
					VSP	S-PLUS
1	0.22	0.22	4.43	3.20	2	2
2	0.06	0.08	3.52	2.66	7	7
3	0.19	0.19	1.19	4.52	51	51
4	0.14	0.13	0.38	2.55	220	220
5	0.07	0.18	0.25	4.28	1677	1677
6	0.12	0.24	2.79	0.86	2	2
7	0.03	0.03	3.02	3.87	26	26
8	0.10	0.21	1.99	7.17	58	58
9	0.05	0.15	3.75	9.87	52	52
10	0.14	0.14	0.94	5.33	151	151
11	0.23	0.24	4.66	6.54	5	5
12	0.23	0.21	4.15	3.16	2	2
13	0.02	0.17	3.79	9.62	61	61
14	0.02	0.16	3.13	6.69	45	45
15	0.14	0.09	3.75	9.21	36	36

Comparisons of Hand Calculations with VSP and S-PLUS When MQO Module Is Not Used

The accuracy of the VSP and S-PLUS calculations was evaluated by also computing the sample-size equations by hand. The hand computations were conducted for 3 of the 15 test cases for each of the statistical tests. The 3 cases for each test were selected so that the computed values of n ranged from very small (less than 10) to very large (more than 1000). The results are provided in Table 3.3. In total, hand calculations were conducted for 27 of the 135 total test cases (15 test cases for each of the 9 statistical tests equals 135). *For all 27 cases, the sample sizes computed by hand were exactly equal to those obtained using the VSP and S-PLUS computer programs.*

Table 3.3. Hand Calculations to Test if VSP Code Accurately Computes Sample Sizes

Statistical Test	Case	Alpha	Beta	Delta [a]	Sd_{total}	Calculated Sample Size		
						VSP	S-PLUS	By Hand
One-sample t-test	1	0.22	0.22	4.43	3.20	2	2	2
	2	0.07	0.18	0.25	4.28	1677	1677	1677
	3	0.02	0.17	3.79	9.62	61	61	61
Wilcoxon signed ranks test	1	0.22	0.22	4.43	3.20	2	2	2
	2	0.07	0.18	0.25	4.28	1946	1946	1946
	3	0.02	0.17	3.79	9.62	71	71	71
One-sample proportion test	1	0.22	0.22	0.289	NA	2	2	2
	2	0.07	0.18	0.02	NA	3407	3407	3407
	3	0.02	0.17	0.37	NA	7	7	7
MARSSIM sign test	1	0.22	0.22	4.43	3.20	4	4	4
	2	0.07	0.18	0.25	4.28	2636	2636	2636
	3	0.02	0.17	3.79	9.62	117	117	117
Confidence interval for mean	1 [b]	0.07	NA	0.64 [c]	8.90	637	637	637
	2 [d]	0.23	NA	0.51 [e]	1.05	4	4	4
	3 [b]	0.27	NA	0.17 [c]	5.72	1379	1379	1379
Two-sample t-test	1	0.22	0.22	4.43	3.20	3	3	3
	2	0.07	0.18	0.25	4.28	3353	3353	3353
	3	0.02	0.17	3.79	9.62	118	118	118
Wilcoxon rank sum test	1	0.22	0.22	4.43	3.20	4	4	4
	2	0.07	0.18	0.25	4.28	3889	3889	3889
	3	0.02	0.17	3.79	9.62	137	137	137
MARSSIM WRS test	1	0.22	0.22	4.43	3.20	4	4	4
	2	0.07	0.18	0.25	4.28	3512	3512	3512
	3	0.02	0.17	3.79	9.62	126	126	126

Table 3.3. Hand Calculations (contd)

Statistical Test	Case	Alpha	Beta	Delta [a]	Sd$_{total}$	Calculated Sample Size		
						VSP	S-PLUS	By Hand
Two-sample test for proportions	1	0.22	0.22	0.44	NA	7	7	7
	2	0.07	0.18	0.03	NA	3062	3062	3062
	3	0.02	0.17	0.38	NA	23	23	23
NA = Not applicable; [a] width of gray region of the Decision Performance Goal Diagram [b] two-sided confidence interval was computed; [c] half-width of two-sided confidence interval [d] one-sided confidence interval was computed; [e] width of one-sided confidence interval.								

Comparisons of Hand Calculations with VSP and S-PLUS When the MQO Module Is Used

The sample-size equations that apply when the MQO module was used were hand-calculated for the following specific cases:

- one-sample t-test [Equation (3.2) for r = 1]
- Wilcoxon signed ranks test [Equation (3.4) for r = 1]
- confidence limit on the mean [Equation (3.10) for r = 2]
- MARSSIM sign test [Equations (3.6) and (3.8) for r = 1 and 2]
- two-sample t-test [Equation (3.12) for r = 2]
- Wilcoxon rank sum test [Equation (3.15) for r = 2]
- MARSSIM WRS test [Equations (3.16) and (3.18) for r = 2]

For each of the above cases, the hand calculation of the sample size agreed exactly with that computed by VSP. However, two problems were identified that were corrected when Version 0.9I of VSP was prepared. The most important discovered was that Version 0.9H of VSP incorrectly displays in some cases the DPGD specified by the VSP user for the MARSSIM sign test and the Wilcoxon rank sum test.

The one-sample and two-sample test for proportions are not included in the above list because the MQO module is not implemented in Version 0.9H of VSP. However, two test cases (hand calculations) were conducted for the one-sample test for proportions for the non-MQO module case. It was found that when the null hypothesis selected was "the site is clean," the VSP program did not correctly compute the sample size. This problem was corrected for Version 0.9I of VSP. Version 0.9H correctly computed the sample size when the null hypothesis selected was "the site is dirty."

3.2.2 Hot Spot Sampling

Davidson (1995a, 1995b) conducted Monte Carlo simulations to verify that the upgraded ELIPGRID-PC program was computing hot-spot detection probabilities correctly. He also compared the computed ELIPGRID-PC detection probabilities with those of 100 test cases published in Singer (1962). *Davidson (1995b) found that his upgraded ELIPGRID-PC program produced probabilities that exactly*

matched those of the 100 test cases. Davidson (2001) applied this same testing procedure to the implementation of ELIPGRID-PC in the VSP software. *He found that the VSP program also gave complete agreement with the 100 test cases in Singer (1962).* These results provide confidence that the ELIPGRID computations in VSP are accurate. The input and output files of these 100 cases are listed in Appendixes C and D, respectively, of Davidson (2001).

3.2.3 Other VSP Outputs

While checking the accuracy of sample-size computations by VSP (Section 3.1), PNNL researchers also checked on the accuracy of the four graphical displays of VSP outputs – the "Map View," the "Graph View," and "Report View," and the "Coordinate View." The Map View shows the locations of the sampling locations at the study site. The Graph View shows the DPGD. The Report View documents the sampling design selected by the VSP user (e.g., simple random sampling), the size of the study site, the recommended minimum number of samples, and the total cost of sampling and measurement. The Coordinate View lists the geographical coordinates of the sampling locations.

As indicated in Section 3.2.1, researchers discovered that VSP displays an incorrect graph of the DPGD for the MARSSIM sign test and the Wilcoxon rank sum test in certain cases. The only other problem discovered was an incomplete listing of all the sample locations in the Coordinate View that occurred for one test case. These problems were corrected for Version 0.9I.

4.0 Verification and Documentation of Nonstatistical Portions of VSP

VSP was designed originally for the Microsoft[(R)] Windows[(R)] 95 operating system, but has been used successfully on several closely related operating systems – Windows[(R)] 95, Windows[(R)] 98, Windows[(R)] Millennium Edition, and Windows[(R)] 2000.

4.1 Installation Success for Various Computer Platforms

Installation and requirements for VSP include:

- IBM-PC compatible desktop or laptop computer with 32 MB or more of RAM.
- Hard drive with 6 MB or more free space.
- Windows 95/98/ME/2000 operating system.

For an installation to be counted as successful, the following ten criteria must be met:

1. The VSP09h.exe setup file must run successfully.
2. VSP options must be available to the user by selecting Start Button 6 Programs 6 Visual Sample Plan.
3. Selection of the VSP Quick-Start Guide (portable document format, or PDF) option should launch Adobe[(R)] Acrobat[(R)] or Acrobat Reader[TM], if available, and display the Quick-Start Guide. If Adobe Acrobat is not available, an appropriate error message should display.
4. Selection of the VSP Quick-Start Guide option should launch Microsoft[(R)] Word[(R)], if available, and display the Quick-Start Guide. If Microsoft Word is not available, an appropriate error message should display.
5. Selection of Start Button 6 Programs 6 Visual Sample Plan 6 Visual Sample Plan should start VSP.
6. The user should be able to click on the Load Map icon labeled DXF and successfully import the Millsite.Dxf file.
7. The user should be able to click on the New Area icon, select a color, and right click inside the top portion of the large oval. The information box should display the area of the oval as 509779.78 Feet^2.
8. The user should then select Sampling Designs 6 Simple Random Sampling 6 Parametric 6 Mean vs. Action Level. Assuming the defaults are Alpha = 5%, Beta = 20%, Delta = 0.25, Action Level = 1, Estimated Standard Deviation = 0.6, the recommended Minimum Samples in Survey Unit should be 37.
9. After closing the Mean vs. Action Level dialog box, the user should be able to save the current project as Test1.vsp using option File 6 Save Project As.

[(R)] Microsoft[(R)], Word[(R)], Windows[(R)] 95, 98, 2000, and Millennium Edition are registered trademarks of Microsoft Corporation, Redmond, Washington.
[(R)] Adobe[(R)], Acrobat[(R)], and Reader[TM] are either trademarks or registered trademarks of Adobe Systems Incorporated, San Jose, California.

10.   After exiting VSP, the user should then be able to restart VSP using option File 6 Open Project open file Test1.vsp. Finally, the user should verify that the same map, oval area, and sample-size of 37 samples for the Mean vs. Action Level option came into VSP.

Table 4.1 documents the results of the installation testing.

Table 4.1. Successful Installations of VSP Version 0.9I

Operating System	Result
Windows 95	Completed successfully [1]
Windows 98	Completed successfully
Windows Me	Completed successfully
Windows 2000	Completed successfully
[1] The VSP Quick-Start in PDF format may not load on all Windows 95 systems. In this case, use the .doc format version with Microsoft Word.	

4.2 Verification of File Import, Export, and Removal of Sampling Locations

One of the key functions of VSP is to overlay random sampling locations on a user's site map. The coordinates for these locations usually are generated by VSP but they also can be imported into a selected study area, exported (saved) to an ASCII text file, or removed from a selected study area. PNNL conducted three tests to verify the import, export, and removal of sampling locations.

A file of 100 random sampling locations (sample points) was generated for the following tests. The X and Y coordinates of each point were allowed to range between 0 and 100.

4.2.1 Import of Sampling Locations

The 100 sample points were loaded into a square sample area that ranged from (0,0) to (100,100). The sample coordinates in the Coordinate View of VSP were compared visually to the original file. All coordinates matched.

4.2.2 Export of Sampling Locations

The 100 sample points were exported to a text file. The coordinates were compared to the original file of random points. All coordinates matched.

4.2.3 Removal of Sampling Locations

The Remove function deletes sample points from the selected sample area if the coordinates match those of the ASCII text file. The remove function was run on the export file of points. All sample points were removed. The remove function was next run on the original file of random points. No

sample points were removed from the sample area. Investigation showed that the function did not work properly on comma-delimited files. The problem was corrected in Version 0.9I, and the function then removed all points using the original file of random points.

4.3 Verification of Drawing Functions

Each drawing function in VSP allows input from the mouse or the keyboard. To test the accuracy of each method of input, researchers used the following procedure for each drawing function:

1. Inputs were made using the mouse, and the points were documented.
2. The same drawing function was performed using the keyboard.
3. The size of the resulting sample area was documented.
4. Visual comparison was made between the two figures.
5. The total size of the two sample areas was confirmed to have doubled.
6. The map was exported to a DXF file, and the coordinates of the figures were compared.

4.3.1 Polyline Drawing Function

The following points were used:

(-72.80,78.00)
(-13.60,26.80)
(20.00, 56.80)
(0,94.00)
(-72.80,78.00) to close
Single-sample area size: 3262.24 square feet
Two-sample area size: 6524.48 square feet

DXF file coordinates matched exactly.

4.3.2 Rectangle Drawing Function

The following corners were used:

(-38.00, 50.00)
(76.80, 93.20)
Single-sample area size: 4959.36 square feet
Two-sample area size: 9918.72 square feet

DXF file coordinates matched exactly.

4.3.3 Ellipse Drawing Function

The following bounding corners were used:

(15.60, 8.80)
(124.40, 76.40)

Single-sample area size: 5739.46 square feet
Two-sample area size: 11478.93 square feet
Note: In VSP, an ellipse is approximated with a series of line segments.

DXF file coordinates matched exactly.

4.3.4 Curve Drawing Function

The following bounding and control points were used:

(6.00, 82.00)
(36.80, 27.20)
(90.00, 78.80)
Single-sample area size: 1181.09 square feet
Two-sample area size: 2362.19 square feet
Notes: In VSP, a curve is approximated with a series of line segments.
        Sample areas are not generated automatically from curves.

DXF file coordinates matched exactly.

4.3.5 MARSSIM Room Drawing Function

The following corner points and wall height were used:

(20.00, 4.00)
(80.00, 34.00)
(8.00)
Single-sample area size: 5040.00 square feet
Two-sample area size: 10080.00 square feet

DXF file coordinates matched exactly.

4.4 Verification of Correspondence Between Dialog Box Values and Values in View Windows

VSP provides the user with four views or windows on the problem at hand – the Report View, Graph View, Map View, and Coordinates View. For a variety of dialog-box input values and dialog-box calculated values, the four VSP views were found to have values that correspond to the dialog-box values.

VSP offers the user many dialog boxes for a variety of options, most of which are related in some way to one of the four views discussed above. An exhaustive test of all possible permutations of dialog box values and the four views was beyond the scope of PNNL's investigation. Instead, two of the most important options were chosen – the one-sample t-test and the two-sample t-test, as examples of VSP's correspondence between dialog box values and view values. A more exhaustive test could possibly be done in the future if a test method were developed that did not depend on the time-intensive process of manually entering the test data into the dialog boxes.

Forty test cases were generated randomly by a MATLAB[(R)] program written for this purpose. These random values were entered manually into the appropriate dialog boxes, and a check was made for exact correspondence between the dialog-box input values, the dialog-box calculated values, and the corresponding value(s) in one of the view windows. All comparisons matched in Version 0.9I. The problems experienced with VSP Version 0.9H are mentioned briefly in the notes to the tables in the next sections.

The MATLAB program code is listed in Appendix B; the random test data are listed in Appendix C.

4.4.1 Dialog Box Values and Report View Values

VSP's Version 0.9I implementation of the Report View was tested by comparing sample size, sampling area, and total sampling cost in the Report View with the corresponding values in a dialog box. All comparisons were identical.

Table 4.2. Tests of Report-View Values Compared with Dialog-Box Values

Case	VSP Option	Null Used	MQO Used	Comparisons
1	One-Sample t-test	Dirty	No	All OK
2	One-Sample t-test	Dirty	Yes	All OK
3	One-Sample t-test	Clean	No	All OK
4	One-Sample t-test	Clean	Yes	All OK
5	One-Sample t-test	Clean	Yes	All OK
6	Two-Sample t-test	Dirty	Yes	All OK
7	Two-Sample t-test	Clean	No	All OK, Note 1
8	Two-Sample t-test	Dirty	No	All OK, Note 1
9	Two-Sample t-test	Clean	No	All OK, Note 1
10	Two-Sample t-test	Clean	Yes	All OK, Note 1

Note 1. VSP Version 0.9H did not allow the specified random delta value to be entered due to a difference in the meaning of the term delta and VSP 0.9H's automatic correction of user input. This problem was corrected in Version 0.9I.

[(R)] MATLAB is a registered trademark of the MathWorks, Inc., Natick, Massachusetts.

4.4.2 Dialog Box Values and Graph View Values

VSP's Version 0.9I implementation of the Graph View was tested by comparing sample size, Alpha, and Beta values in the Graph View with the corresponding values in a dialog box. All comparisons were identical.

Table 4.3. Tests of Graph-View Values Compared with Dialog-Box Values

Case	VSP Option	Null Used	MQO Used	Comparisons
1	One-Sample t-test	Dirty	No	All OK
2	One-Sample t-test	Dirty	Yes	All OK
3	One-Sample t-test	Clean	No	All OK
4	One-Sample t-test	Clean	Yes	All OK
5	One-Sample t-test	Clean	Yes	All OK
6	Two-Sample t-test	Dirty	Yes	All OK, Note 1
7	Two-Sample t-test	Clean	No	All OK, Notes 1, 2
8	Two-Sample t-test	Dirty	No	All OK, Notes 1, 2
9	Two-Sample t-test	Clean	No	All OK, Notes 1, 2
10	Two-Sample t-test	Clean	Yes	All OK, Notes 1, 2

Note 1. In VSP Version 0.9H, the Decision Performance Goal Diagram did not show the alpha and beta error rates in the subtitle of the graph. This problem was corrected in Version 0.9I.

Note 2. VSP Version 0.9H did not allow the specified random delta value to be entered due to a difference in the meaning of the term delta and VSP 0.9H's automatic correction of user input. This problem was corrected in Version 0.9I.

4.4.3 Dialog Box Values and Map View Values

VSP's Version 0.9I implementation of the Map View was tested by comparing the recommended sample size given in the dialog box with the number of sampling locations actually plotted on the map. All comparisons were identical.

Table 4.4. Tests of Map-View Values Compared with Dialog-Box Values

Case	VSP Option	Null Used	MQO Used	Comparisons
1	One-Sample t-test	Clean	No	All OK
2	One-Sample t-test	Dirty	Yes	All OK
3	One-Sample t-test	Clean	No	All OK
4	One-Sample t-test	Clean	Yes	All OK
5	One-Sample t-test	Dirty	No	All OK
6	Two-Sample t-test	Dirty	Yes	All OK
7	Two-Sample t-test	Clean	Yes	All OK
8	Two-Sample t-test	Clean	Yes	All OK
9	Two-Sample t-test	Dirty	Yes	All OK
10	Two-Sample t-test	Dirty	No	All OK

4.4.4 Dialog Box Values and Coordinate View Values

The VSP Version 0.9I implementation of the Coordinate View was tested by comparing the recommended sample size given in the dialog box with the number of sampling-location coordinate pairs actually listed in the Coordinate View. All comparisons were identical.

Table 4.5. Tests of Map-View Values Compared with Dialog-Box Values

Case	VSP Option	Null Used	MQO Used	Comparison[1]
1	One-Sample t-test	Clean	No	All OK, Note l
2	One-Sample t-test	Dirty	Yes	All OK, Note l
3	One-Sample t-test	Clean	No	All OK, Note l
4	One-Sample t-test	Clean	Yes	All OK, Note l
5	One-Sample t-test	Dirty	No	All OK, Note l
6	Two-Sample t-test	Dirty	Yes	All OK, Note l
7	Two-Sample t-test	Clean	Yes	All OK, Note l
8	Two-Sample t-test	Clean	Yes	All OK, Note l
9	Two-Sample t-test	Dirty	Yes	All OK, Note l
10	Two-Sample t-test	Dirty	No	All OK, Note l

Note 1. For at least one of the above cases, VSP Version 0.9H did not allow the specified random delta value to be entered due to a difference in the meaning of the term delta and VSP 0.9H's automatic correction of user input. Testing of Version 0.9H was stopped before this table was completed. This problem was corrected in Version 0.9I.

4.5 Documentation of Algorithms to Determine Sampling Locations

The VSP user can choose from four methods that determine sampling locations. The three methods documented here produce sampling locations based on algorithms in VSP. The user also can manually select arbitrary sampling locations using the option Sampling Designs / Judgment Sampling / Manually Add Samples. Only the three computer-based methods are documented here.

4.5.1 Regular Simple Random Sampling Algorithm

Regular simple random samples are placed in the sample area by choosing one of the sampling designs listed on the Sampling Designs / Simple Random Sampling menu. The placement option should be set to Regular Random on the Options / Sample Placement menu (this is the default setting).

Using this method, each sample is placed according to the following algorithm without regard to existing samples:

1.   randomx and randomy values are obtained using the chosen random number generator (described above). These random values are fractions between 0 and 1.
2.   The sample point coordinates are calculated by the following formulas:

$$x = XMin + (Xmax - XMin) * randomx$$
$$y = YMin + (Ymax - YMin) * randomy$$

where

x = x coordinate of sample
y = y coordinate of sample
XMin = minimum x extent of sample area
XMax = maximum x extent of sample area
YMin = minimum y extent of sample area
YMax = maximum y extent of sample area

3.   The sample location (x, y) is checked to make sure it lies inside the sample area. If it does, a new sample point is added at the location. If not, another random location is tried.

For multiple Sample Areas, the number of samples assigned to each sample area is calculated by the following formula:

$$n = floor(samples * area / total)$$

where

n = number of samples to be assigned to the current Sample Area
floor() = function that returns the largest whole number less than or equal to a number
samples = total number of samples to be assigned to all Sample Areas
area = surface area of current Sample Area
total = total surface area of all Sample Areas

If the formula leaves unassigned samples (because of rounding down), one sample is added to each Sample Area in turn, until all remaining samples are placed.

4.5.2 Adaptive-Fill Simple Random Sampling Algorithm

Adaptive fill samples are placed in the sample area by choosing one of the sampling designs listed on the Sampling Designs / Simple Random Sampling menu. The placement option must be set to Adaptive Fill on the Options / Sample Placement menu.

Using this method, samples are placed according to the following algorithm:

1.   An initial spacing value is calculated using the following equation:

$$spacing = sqrt(area / samples)$$

where

spacing = the initial spacing value
sqrt() = the square root function
area = the surface area of the Sample Area
samples = the number of samples to place

Then Steps 2 through 4 are performed once for each sample to be placed:

2.	A sample location is obtained using the algorithm described in Regular Random.
3.	The existing sample closest to the new sample location is found.
4.	If the distance to the closest sample is greater than the spacing value the sample is added.
5.	If not all samples were placed, then the spacing value is multiplied by 0.99 and Steps 2 through 4 are repeated for each remaining sample. If all samples were placed, then the algorithm is finished.

For multiple Sample Areas, a spacing value is calculated for each Sample Area, and the largest one is used as the initial spacing value. Each Sample Area is given a chance to place all the samples (Steps 2 through 4). The total number of samples placed is tracked, and the next Sample Area is given an opportunity to place the remaining samples. Processing continues with Step 5 after each Sample Area is given a chance to place samples.

4.5.3 Systematic Grid Sampling Algorithm

Grid samples are placed in the sample area by choosing one of the sampling designs listed on the Sampling Designs / Systematic Grid Sampling menu.

Using this method, samples are placed according to the following algorithm:

1.	The bounding box of the Sample Area is surrounded by a larger bounding box that is tilted at the angle specified by the user. The upper left corner of this box is found by the following formulas:

$$x = XMin - \cos(angle) * length$$
$$y = YMin + \sin(angle) * length$$

where

x = x coordinate of tilted box
y = y coordinate of tilted box
angle = angle of tilt specified by user
XMin = minimum x extent of Sample Area
YMin = minimum y extent of Sample Area
$\cos()$ = cosine function
$\sin()$ = sine function
$$length = (YMax - YMin) * \sin(angle)$$

where

YMax = maximum y extent of Sample Area

2.	If a random start grid is selected by the user, then a random offset is subtracted from the corner point.
For rectangular grids:

$$xx = x - size * random$$
$$yy = y - size2 * random2$$

For square and triangular grids:

$$xx = x - size * random$$
$$yy = y - size * random2$$

where

xx = offset x coordinate of tilted box
yy = offset y coordinate of tilted box
size = length of side of grid

4.10

size2 = length of other side of rectangular grid

random = a random number supplied by one of the random number generators

random2 = a random number supplied by one of the random number generators.

3.   The number of grid columns across the sample area is calculated by the following formula:

columns = int((length + length2) / size + 1.0)

where

columns = the number of columns across the Sample Area grid

int() = truncation function

length2 = (XMax - XMin) * sin(PI / 2.0 - angle)

where

XMax = maximum x extent of Sample Area

PI = 3.1415926535

4.   The number of grid rows down the sample area is calculated by the following formulas:

For square grids:

rows = int((length3 + length4) / size + 1.0)

For triangular grids:

rows = int((length3 + length4) / (sin(PI / 3.0) * size * 2.0) + 1.0)

For rectangular grids:

rows = int((length3 + length4) / size2 + 1.0)

where

rows = number of rows down the Sample Area grid

length3 = (YMax - YMin) * sin(PI / 2.0 - angle)

length4 = (XMax - XMin) * sin(angle)

5.   If random start is specified by the user, rows and columns are incremented by 2 to ensure complete coverage of the Sample Area.

6.   The distances to move for each row are calculated by the following formulas:

For square grids:

rxdelta = cos(PI / 2.0 - angle) * size

rydelta = sin(PI / 2.0 - angle) * size

For triangular grids:

rxdelta = cos(PI / 2.0 - angle) * (sin(PI / 3.0) * size)

rydelta = sin(PI / 2.0 - angle) * (sin(PI / 3.0) * size)

For rectangular grids:

rxdelta = cos(PI / 2.0 - angle) * size2

rydelta = sin(PI / 2.0 - angle) * size2

where

rxdelta = amount to move x coordinate for each row

rydelta = amount to move y coordinate for each row

7.   The distances to move for each column are calculated by the following formulas:

cxdelta = cos(angle) * size

cydelta = -sin(angle) * size

where

cxdelta = amount to move x coordinate for each column

cydelta = amount to move y coordinate for each column

8.   Sample points are then placed according to the following algorithms:
       For square and rectangular grids:
       a.   The first sample point is (x,y)
       b.   The sample point is checked to see if it is inside the Sample Area. If so, the sample point is added to the Sample Area. If not, it is discarded
       c.   The next sample point is the next column located at (x+cxdelta, y+cydelta). Steps b and c continue until all the columns have been checked.
       d.   The next sample point is the next row located at (x+rxdelta, y+rydelta). Steps b through d continue until all the rows have been checked.
       For triangular grids:
       a.   The first sample point is (x,y)
       b.   The sample point is checked to see if it is inside the Sample Area. If so, the sample point is added to the Sample Area. If not, it is discarded.
       c.   The next sample point is the next column located at (x+cxdelta, y+cydelta). Steps b and c continue until all the columns have been checked.
       d.   Even numbered rows are offset by one row and by half a column width (x+rxdelta+cxdelta/2, y+rydelta+cydelta/2). Odd numbered rows are offset by one row and no columns (x+rxdelta, y+rydelta). Steps b through d continue until all the rows have been checked.

4.6 Documentation of Random Number Generators

VSP users can choose between two random number generators for placement of samples by making a selection from the Options / Random Numbers menu. This section documents the algorithms used in VSP for these important functions.

4.6.1 Pseudo-Random Number Generator

The pseudo-random number generator produces a sequence of numbers using the following algorithm:

1.   value = previous seed * 16807.0
2.   seed = value MODULO 2147483647.0
3.   random number = seed / 2147483647.0

The initial seed is set to 1.0 when a sample area is created. The seed value is preserved after each random number is produced.

This algorithm is based on a minimal standard random number generator recommended by Park and Miller (1988) and used for the Monte Carlo simulation tests of the ELIPGRID-PC algorithm by Davidson (1995).

4.6.2 Quasi-Random Number Generator

This algorithm is based on Halton's Sequence discussed in Press et al. (1992, p. 300). The basic idea is to generate random sampling locations that avoid each other and yet still randomly fill the space. Conceptually, one can think of electrons in a box. At any moment, each electron is in a random location but they all are avoiding other electrons because of like negative charges. In contrast, a pseudo-random number generator is not constrained from generating lists of X, Y coordinates with locations very near other locations.

The quasi-random number generator produces a sequence of paired (X, Y) numbers using the following algorithm:

1. An integer value, iSeq, is used as the basis of the algorithm
    (e.g., 457)
2. iSeq is expressed as a 32 digit binary number
    (e.g., bSeq = 00000000000000000000000111001001)
3. The sequence of digits is reversed
    (e.g., rbSeq = 10010011100000000000000000000000)
4. The sequence of digits is again expressed as a decimal integer
    (e.g., xVal = 2474639360)
5. xVal is converted to a fraction by dividing by 4294967295.0
    (e.g., X = 0.576171875)
6. iSeq is expressed as a 20 digit base 3 number
    (e.g., tSeq = 00000000000000121221)
7. The sequence of digits is reversed
    (e.g., rtSeq = 12212100000000000000)
8. The sequence of digits is again expressed as a decimal integer
    (e.g., yVal = 2271910275)
9. yVal is converted to a fraction by dividing by 4294967295.0
    (e.g., Y = 0.52897033)
10. The values X and Y are used as the random pair.

iSeq is initially set to 1. It is incremented by 1, and the value is preserved after each usage.

5.0 References

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Appendix A

Peer Review Comments on Sample-Size Equations in VSP

Appendix A

Peer Review Comments on Sample-Size Equations in VSP

by

Robert F. O'Brien
Statistics Group, Pacific Northwest National Laboratory
Richland, Washington

October 16, 2000

1. Sample sizes for the t-test are obtained by using standard normal values of $Z_{1-\alpha}$ and $Z_{1-\beta}$. This is fine for larger sample sizes. However, where the t-test is most applicable, for smaller sample sizes, I think it would be more appropriate to use $t_{1-\alpha}$ and $t_{1-\beta}$ and then iterate to the correct sample accounting for the degrees of freedom.

2. The sample size formula for the WRS test is suspect to me. It assumes the asymptotic normality of the test statistic. For small sample sizes, this could give spurious results. I would like to see some simulations run to support the use of this sample size formula for both large and small sample sizes.

3. When discussing the nonparametric tests, be careful when a mean is appropriate and when a median is appropriate. A mean is equivalent to a median only if the underlying distribution is symmetric. And if the underlying distribution is symmetric, a normal distribution will probably fit in most cases.

4. Sample size output validation should be verified by someone other than I.

Appendix B

Listing of MATLAB Code for Program Used in Section 3.4

Appendix B

Listing of MATLAB Code for Program Used To Verify Correspondence Between Dialog Box Values and Values in View Windows

```
function VSPNonStatTests(FileName)
%VSPNONSTATTESTS  Writes a test data file for VSP non-stat tests.
%  Usage:         VSPNonStatTests[(FileName)]
%  Examples:      VSPNonStatTest               % NonStatTests.Dat is default.
%                 VSPNonStatTest('Test1.Dat')  % Test1.Dat is output file.
%  Notes:         This program is designed to provide random test data for VSP
%                 that is appropriate to the various input dialog boxes and
%                 VSP's four View windows.


%  Started:    01/09/2001
%  Last Mod:   01/29/2001
%  Language:   MATLAB Version 5.3
%  Author:     Jim Davidson, Davidson and Davidson, Inc.
%  Contract:   Battelle Contract 406437-A-A5

FOPEN_ERROR        = -1;
VSP_VERSION        = '0.9i';
MATLAB_VERSION     = '5.3';
PROG_VERSION       = '01/29/2001';

MAX_TRIALS         = 5;
MAX_ALPHA          = 20;
MAX_BETA           = 50;
MAX_ACTION_LEVEL   = 200;
MAX_COST           = 1000;

if nargin == 0
   FileName = 'NonStatTests.Dat';
end

fid = fopen(FileName, 'wt');
if fid == FOPEN_ERROR
   disp(['Error: Can not open file ' FileName]);
   return;
end

disp([' --- Running VSPNonStatTests Version ' PROG_VERSION ' ---']);
disp(['Writing file: ' FileName]);

% Write the heading to the output file
fprintf(fid, 'File:           %s\n', FileName);
fprintf(fid, 'Purpose:        %s\n',...
   'Provides random test data for VSP non-stat tests');
fprintf(fid, 'Produced by:    %s\n',...
   ['VSPNonStatTest program, Version ', PROG_VERSION]);
fprintf(fid, 'VSP Version:    %s\n', VSP_VERSION);
fprintf(fid, 'MATLAB Version: %s\n', MATLAB_VERSION);
fprintf(fid, 'Date:           %s\n', Today);

%---These tests are designed for the Report and Graph Views.
%---They can have both small and large random sample sizes.
TableNo = 1;
fprintf(fid,...
```

```
    ['\n\n Table ' num2str(TableNo) '. '...
    'Random Data to Compare One-Sample t-Test Dialog Box and Report and '...
    'Graph Views in VSP\n']);
fprintf(fid, [rep('-', 123) '\n']);
fprintf(fid, [' Null Alpha  Beta     Delta ActnLevel   TotalSD SmplingSD ',...
    ' MsrmntSD Reps  SampSize FixedCost  FieldCost MeasCost  TotalCost\n']);
fprintf(fid, ['----- ----- ----- --------- --------- --------- --------- ',...
    '--------- ---- --------- --------- ---------- -------- ----------\n']);
TableNo = TableNo + 1;

% Make the random number generator go to same state each time this is run
rand('state', 0);
for Trial = 1:MAX_TRIALS
    if rand < .5, Null = 'Clean'; else Null = 'Dirty'; end;
    % Num2Digits is used to make sure the values used by this program are the
    % same as the values typed into VSP
    Alpha          = Num2Digits(1 + rand * MAX_ALPHA/2, 1);
    Beta           = Num2Digits(1 + rand * MAX_BETA/2, 1);
    ActionLevel    = Num2Digits(rand * MAX_ACTION_LEVEL, 1);
    Delta          = Num2Digits(rand * ActionLevel, 1);
    StdDev         = Num2Digits(rand * 10 * Delta, 1);

    ZOneMinusAlpha = norminv(1-Alpha/100);
    ZOneMinusBeta  = norminv(1-Beta/100);

    if rand < .5
        UseMQO         = 'N';
        Reps           = 1;
        StdDevSq       = StdDev^2;
    else
        UseMQO         = 'Y';
        % Make Reps 1, 2, or 3
        if rand < .333, Reps = 1; else Reps = 2; end;
        if Reps == 2 & rand > .5, Reps = 3; end;
        SamplingStdDev = Num2Digits(rand * StdDev, 1);
        MeasStdDev     = Num2Digits(rand * StdDev, 1);
        StdDevSq       = SamplingStdDev^2 + MeasStdDev^2/Reps;
    end;

    SampSize    = StdDevSq * ((ZOneMinusAlpha + ZOneMinusBeta)^2/Delta^2)...
        + 0.5 * ZOneMinusAlpha^2;
    SampSize    = ceil(SampSize);
    FixedCost   = Num2Cur(rand * MAX_COST);
    FieldCost   = Num2Cur(rand * MAX_COST);
    MeasCost    = Num2Cur(rand * MAX_COST);
    TotalCost   = FixedCost + FieldCost * SampSize + Reps * SampSize * MeasCost;

    if UseMQO == 'N'
        fprintf(fid, ['%5s%6.1f%6.1f%10.1f%10.1f%10.1f%10s%10s%5.1f',...
            '%10.0f%10s%10s%10s%11s\n'],...
            Null, Alpha, Beta, Delta, ActionLevel, StdDev, 'N/A', 'N/A', Reps',...
            SampSize, Num2CurStr(FixedCost), Num2CurStr(FieldCost),...
            Num2CurStr(MeasCost), Num2CurStr(TotalCost));
    else
        % If here, Use MQO
        fprintf(fid, ['%5s%6.1f%6.1f%10.1f%10.1f%10s%10.1f%10.1f%5.1f',...
            '%10.0f%10s%10s%10s%11s\n'],...
            Null, Alpha, Beta, Delta, ActionLevel, 'N/A', SamplingStdDev,...
            MeasStdDev, Reps,...
            SampSize, Num2CurStr(FixedCost), Num2CurStr(FieldCost),...
            Num2CurStr(MeasCost), Num2CurStr(TotalCost));
    end
end;

%---These tests are designed for the Map and Coord. Views.
```

```
%---Thus they have small random sample sizes usually between 1 and 20.
fprintf(fid,...
    ['\n\n Table ' num2str(TableNo) '. '...
    'Random Data to Compare One-Sample t-Test Dialog Box and Map and '...
    'Coordinate Views in VSP\n']);
fprintf(fid, [rep('-', 123) '\n']);
fprintf(fid, [' Null Alpha  Beta    Delta ActnLevel   TotalSD SmplingSD ',...
    ' MsrmntSD Reps  SampSize FixedCost  FieldCost MeasCost  TotalCost\n']);
fprintf(fid, ['----- ----- ----- --------- --------- --------- --------- ',...
    '--------- ---- --------- --------- ---------- -------- ----------\n']);
TableNo = TableNo + 1;

for Trial = 1:MAX_TRIALS
    if rand < .5, Null = 'Clean'; else Null = 'Dirty'; end;
    % Note that Alpha and Beta below are kept large to reduce sample sizes
    % Num2Digits is used to make sure the values used by this program are the
    % same as the values typed into VSP
    Alpha           = Num2Digits(10 + rand * MAX_ALPHA, 1);
    Beta            = Num2Digits(10 + rand * MAX_BETA, 1);
    ActionLevel     = Num2Digits(rand * MAX_ACTION_LEVEL, 1);
    Delta           = Num2Digits(rand * ActionLevel, 1);
    % Note that SdtDev below is kept small to reduce sample sizes
    StdDev          = Num2Digits(rand * Delta + .7 * Delta, 1);

    ZOneMinusAlpha = norminv(1-Alpha/100);
    ZOneMinusBeta  = norminv(1-Beta/100);

    if rand < .5
        UseMQO          = 'N';
        Reps            = 1;
        StdDevSq        = StdDev^2;
    else
        UseMQO          = 'Y';
        % Make Reps 1, 2, or 3
        if rand < .333, Reps = 1; else Reps = 2; end;
        if Reps == 2 & rand > .5, Reps = 3; end;
        SamplingStdDev = Num2Digits(rand * StdDev, 1);
        MeasStdDev     = Num2Digits(rand * StdDev, 1);
        StdDevSq       = SamplingStdDev^2 + MeasStdDev^2/Reps;
    end;

    SampSize    = StdDevSq * ((ZOneMinusAlpha + ZOneMinusBeta)^2/Delta^2)...
        + 0.5 * ZOneMinusAlpha^2;
    SampSize    = ceil(SampSize);
    FixedCost   = Num2Cur(rand * MAX_COST);
    FieldCost   = Num2Cur(rand * MAX_COST);
    MeasCost    = Num2Cur(rand * MAX_COST);
    TotalCost   = FixedCost + FieldCost * ceil(SampSize) + Reps * ...
        ceil(SampSize) * MeasCost;

    if UseMQO == 'N'
        fprintf(fid, ['%5s%6.1f%6.1f%10.1f%10.1f%10.1f%10s%10s%5.1f',...
            '%10.0f%10s%10s%10s%11s\n'],...
            Null, Alpha, Beta, Delta, ActionLevel, StdDev, 'N/A', 'N/A', Reps',...
            SampSize, Num2CurStr(FixedCost), Num2CurStr(FieldCost),...
            Num2CurStr(MeasCost), Num2CurStr(TotalCost));
    else
        % If here, Use MQO
        fprintf(fid, ['%5s%6.1f%6.1f%10.1f%10.1f%10s%10.1f%10.1f%5.1f',...
            '%10.0f%10s%10s%10s%11s\n'],...
            Null, Alpha, Beta, Delta, ActionLevel, 'N/A', SamplingStdDev,...
            MeasStdDev, Reps,...
            SampSize, Num2CurStr(FixedCost), Num2CurStr(FieldCost),...
            Num2CurStr(MeasCost), Num2CurStr(TotalCost));
    end
```

B.3

```
end;

%---These tests are designed for the Report and Graph Views.
%---They can have both small and large random sample sizes.
fprintf(fid,...
    ['\n\n Table ' num2str(TableNo) '. '...
    'Random Data to Compare Two-Sample t-Test Dialog Box and Report and '...
    'Graph Views in VSP\n']);
fprintf(fid, [rep('-', 123) '\n']);
fprintf(fid, [' Null Alpha  Beta     Delta ActnLevel   TotalSD SmplingSD ',...
    ' MsrmntSD Reps  SampSize FixedCost  FieldCost MeasCost  TotalCost\n']);
fprintf(fid, ['----- ----- ----- -------- -------- --------- --------- ',...
    '--------- ---- -------- --------- ---------- -------- ----------\n']);
TableNo = TableNo + 1;

for Trial = 1:MAX_TRIALS
    if rand < .5, Null = 'Clean'; else Null = 'Dirty'; end;
    % Num2Digits is used to make sure the values used by this program are the
    %  same as the values typed into VSP
    Alpha        = Num2Digits(1 + rand * MAX_ALPHA/2, 1);
    Beta         = Num2Digits(1 + rand * MAX_BETA/2, 1);
    ActionLevel  = Num2Digits(rand * MAX_ACTION_LEVEL, 1);
    Delta        = Num2Digits(rand * ActionLevel, 1);
    StdDev       = Num2Digits(rand * 10 * Delta, 1);

    ZOneMinusAlpha = norminv(1-Alpha/100);
    ZOneMinusBeta  = norminv(1-Beta/100);

    if rand < .5
        UseMQO       = 'N';
        Reps         = 1;
        StdDevSq     = StdDev^2;
    else
        UseMQO       = 'Y';
        % Make Reps 1, 2, or 3
        if rand < .333, Reps = 1; else Reps = 2; end;
        if Reps == 2 & rand > .5, Reps = 3; end;
        SamplingStdDev = Num2Digits(rand * StdDev, 1);
        MeasStdDev     = Num2Digits(rand * StdDev, 1);
        StdDevSq       = SamplingStdDev^2 + MeasStdDev^2/Reps;
    end;

    SampSize    = 2 * StdDevSq * ((ZOneMinusAlpha + ZOneMinusBeta)^2/Delta^2)...
        + 0.25 * ZOneMinusAlpha^2;
    SampSize    = ceil(SampSize);
    FixedCost   = Num2Cur(rand * MAX_COST);
    FieldCost   = Num2Cur(rand * MAX_COST);
    MeasCost    = Num2Cur(rand * MAX_COST);
    TotalCost   = FixedCost + FieldCost * SampSize + Reps * SampSize * MeasCost;

    if UseMQO == 'N'
        fprintf(fid, ['%5s%6.1f%6.1f%10.1f%10.1f%10.1f%10s%10s%5.1f',...
            '%10.0f%10s%10s%10s%11s\n'],...
            Null, Alpha, Beta, Delta, ActionLevel, StdDev, 'N/A', 'N/A', Reps',...
            SampSize, Num2CurStr(FixedCost), Num2CurStr(FieldCost),...
            Num2CurStr(MeasCost), Num2CurStr(TotalCost));
    else
        % If here, Use MQO
        fprintf(fid, ['%5s%6.1f%6.1f%10.1f%10.1f%10s%10.1f%10.1f%5.1f',...
            '%10.0f%10s%10s%10s%11s\n'],...
            Null, Alpha, Beta, Delta, ActionLevel, 'N/A', SamplingStdDev,...
            MeasStdDev, Reps,...
            SampSize, Num2CurStr(FixedCost), Num2CurStr(FieldCost),...
            Num2CurStr(MeasCost), Num2CurStr(TotalCost));
    end
```

B.4

```
end;

%---These tests are designed for the Map and Coord. Views.
%---Thus they have small random sample sizes usually between 1 and 20.
fprintf(fid,...
    ['\n\n Table ' num2str(TableNo) '. '...
    'Random Data to Compare Two-Sample t-Test Dialog Box and Map and '...
    'Coordinate Views in VSP\n']);
fprintf(fid, [rep('-', 123) '\n']);
fprintf(fid, [' Null Alpha  Beta    Delta ActnLevel   TotalSD SmplingSD ',...
    ' MsrmntSD Reps  SampSize FixedCost  FieldCost MeasCost  TotalCost\n']);
fprintf(fid, ['----- ----- ----- -------- -------- --------- --------- ',...
    '--------- ---- --------- --------- ---------- -------- ----------\n']);
TableNo = TableNo + 1;

for Trial = 1:MAX_TRIALS
    if rand < .5, Null = 'Clean'; else Null = 'Dirty'; end;
    % Note that Alpha and Beta below are kept large to reduce sample sizes
    % Num2Digits is used to make sure the values used by this program are the
    %  same as the values typed into VSP
    Alpha       = Num2Digits(10 + rand * MAX_ALPHA, 1);
    Beta        = Num2Digits(10 + rand * MAX_BETA, 1);
    ActionLevel = Num2Digits(rand * MAX_ACTION_LEVEL, 1);
    Delta       = Num2Digits(rand * ActionLevel, 1);
    % Note that SdtDev below is kept small to reduce sample sizes
    StdDev      = Num2Digits(rand * Delta + .7 * Delta, 1);

    ZOneMinusAlpha = norminv(1-Alpha/100);
    ZOneMinusBeta  = norminv(1-Beta/100);

    if rand < .5
        UseMQO      = 'N';
        Reps        = 1;
        StdDevSq    = StdDev^2;
    else
        UseMQO      = 'Y';
        % Make Reps 1, 2, or 3
        if rand < .333, Reps = 1; else Reps = 2; end;
        if Reps == 2 & rand > .5, Reps = 3; end;
        SamplingStdDev = Num2Digits(rand * StdDev, 1);
        MeasStdDev     = Num2Digits(rand * StdDev, 1);
        StdDevSq       = SamplingStdDev^2 + MeasStdDev^2/Reps;
    end;

    SampSize    = 2 * StdDevSq * ((ZOneMinusAlpha + ZOneMinusBeta)^2/Delta^2)...
        + 0.25 * ZOneMinusAlpha^2;
    SampSize    = ceil(SampSize);
    FixedCost   = Num2Cur(rand * MAX_COST);
    FieldCost   = Num2Cur(rand * MAX_COST);
    MeasCost    = Num2Cur(rand * MAX_COST);
    TotalCost   = FixedCost + FieldCost * ceil(SampSize) + Reps *...
    ceil(SampSize) * MeasCost;

    if UseMQO == 'N'
        fprintf(fid, ['%5s%6.1f%6.1f%10.1f%10.1f%10.1f%10s%10s%5.1f',...
            '%10.0f%10s%10s%10s%11s\n'],...
            Null, Alpha, Beta, Delta, ActionLevel, StdDev, 'N/A', 'N/A', Reps',...
            SampSize, Num2CurStr(FixedCost), Num2CurStr(FieldCost),...
            Num2CurStr(MeasCost), Num2CurStr(TotalCost));
    else
        % If here, Use MQO
        fprintf(fid, ['%5s%6.1f%6.1f%10.1f%10.1f%10s%10.1f%10.1f%5.1f',...
            '%10.0f%10s%10s%10s%11s\n'],...
            Null, Alpha, Beta, Delta, ActionLevel, 'N/A', SamplingStdDev,...
            MeasStdDev, Reps,...
```

B.5

```
        SampSize, Num2CurStr(FixedCost), Num2CurStr(FieldCost),...
        Num2CurStr(MeasCost), Num2CurStr(TotalCost));
   end
end;

fclose(fid);
disp(['End run: VSPNonStatTests...']);
return;
%%% End of Func: VSPNonStatTests

%-------------------------------------------------------------------------------
function Result = Num2Cur(Num)
% Num2Cur returns Num as a number with two sig. digits to right of dec. point.
% Example: Num2Cur(123.123) ===> 123.12

Result = str2num(num2str(Num, '%.2f'));
return
%%% End of Func: Num2Cur

%-------------------------------------------------------------------------------
function Result = Num2Digits(Num, NumDigits)
% Num2Digits returns Num as a number with NumDigits to right of decimal point.
% Example: Num2Digits(123.123, 1) ===> 123.1

Result = str2num(num2str(Num, ['%.' num2str(NumDigits) 'f']));
return
%%% End of Func: Num2Digits

%-------------------------------------------------------------------------------
function Result = Num2CurStr(Num)
% Num2CurStr returns Num in *.DD currency string format.
% Example: Num2CurStr(123.123) ===> '123.12'

Result = num2str(Num, '%.2f');
return
%%% End of Func: Num2CurStr

%-------------------------------------------------------------------------------
function Result = Today
% Today returns date today as string, based on HMSToday code.
% Example: Today ==> '09/18/2000'

YearMonthDay  = clock;
Result        = strcat(num2str(YearMonthDay(2)), '/',...
   num2str(YearMonthDay(3)), '/', num2str(YearMonthDay(1)));
% Modify single digit month, e.g., 9/12/2000 to 09/12/2000
if Result(2) == '/'
   Result = ['0' Result];
end
%%% End of Func: Today

%%% End of File: VSPNonStatTests.m
```

B.6

Appendix C

Listing of Random Test Data for Section 3.4

Appendix C

Listing of Random Test Data for Verification of Correspondence Between Dialog Box Values and Values in View Windows

```
File:           NonStatTests.Dat
Purpose:        Provides random test data for VSP non-stat tests
Produced by:    VSPNonStatTest program, Version 01/29/2001
VSP Version:    0.9i
MATLAB Version: 5.3
Date:           01/29/2001
```

Table 1. Random Data to Compare One-Sample t-Test Dialog Box and Report and Graph Views in VSP

-

Null	Alpha	Beta	Delta	ActnLevel	TotalSD	SmplingSD	MsrmntSD	Reps	SampSize	FixedCost	FieldCost	MeasCost TotalCost
Dirty	3.3	16.2	86.6	97.2	660.0	N/A	N/A	1.0	466	18.50	821.41	444.70 590025.76
Dirty	8.9	24.0	26.0	147.6	N/A	94.3	6.1	2.0	57	352.87	813.17	9.86 47827.60
Clean	3.0	6.0	32.9	120.8	65.4	N/A	N/A	1.0	49	746.79	445.10	931.81 68215.38
Clean	5.2	22.2	21.3	105.0	N/A	97.6	54.3	1.0	159	831.80	502.81	709.47 193584.32
Clean	4.0	5.7	26.4	38.7	N/A	55.8	30.2	1.0	66	860.01	853.66	593.56 96376.53

Table 2. Random Data to Compare One-Sample t-Test Dialog Box and Map and Coordinate Views in VSP

-

Null	Alpha	Beta	Delta	ActnLevel	TotalSD	SmplingSD	MsrmntSD	Reps	SampSize	FixedCost	FieldCost	MeasCost TotalCost
Clean	28.0	51.1	105.5	129.0	143.5	N/A	N/A	1.0	1	289.73	341.19	534.08 1165.00
Dirty	16.2	51.9	42.1	113.6	N/A	36.7	47.0	3.0	2	956.84	522.59	880.14 7282.86
Clean	29.6	23.6	44.2	50.5	63.5	N/A	N/A	1.0	4	11.76	893.90	199.14 4383.92
Clean	23.2	24.2	6.1	93.8	N/A	3.4	4.5	3.0	2	225.95	579.81	760.37 5947.79

C.1

Null	Alpha	Beta	Delta	ActnLevel	TotalSD	SmplingSD	MsrmntSD	Reps	SampSize	FixedCost	FieldCost	MeasCost	TotalCost
Dirty	22.8	20.5	59.5	76.0	82.2	N/A	N/A	1.0	5	567.83	794.21	59.18	4834.78

Table 3. Random Data to Compare Two-Sample t-Test Dialog Box and Report and Graph Views in VSP

Null	Alpha	Beta	Delta	ActnLevel	TotalSD	SmplingSD	MsrmntSD	Reps	SampSize	FixedCost	FieldCost	MeasCost	TotalCost
Dirty	1.5	11.4	53.3	61.0	N/A	6.3	3.5	3.0	2	498.31	213.96	643.49	4787.17
Clean	10.6	19.2	61.4	82.4	164.5	N/A	N/A	1.0	65	933.38	683.33	212.56	59166.23
Dirty	7.3	4.3	25.1	41.4	158.1	N/A	N/A	1.0	799	575.15	451.42	43.90	396335.83
Clean	4.1	1.3	52.5	76.8	48.7	N/A	N/A	1.0	28	612.40	608.54	15.76	18092.80
Clean	2.9	15.7	4.2	11.5	N/A	12.0	11.7	2.0	204	353.25	153.61	675.64	307350.81

C.2

Table 4. Random Data to Compare Two-Sample t-Test Dialog Box and Map and Coordinate Views in VSP

Null	Alpha	Beta	Delta	ActnLevel	TotalSD	SmplingSD	MsrmntSD	Reps	SampSize	FixedCost	FieldCost	MeasCost	TotalCost
Dirty	24.6	33.9	13.4	111.0	N/A	3.9	13.3	2.0	2	232.35	804.87	908.40	5475.69
Clean	14.8	12.5	10.1	15.7	N/A	1.5	8.9	1.0	8	439.79	340.05	314.22	5673.95
Clean	17.9	39.6	0.9	23.9	N/A	0.2	0.9	2.0	2	237.88	645.83	966.89	5397.10
Dirty	27.4	10.5	22.4	27.4	N/A	8.8	4.2	3.0	2	155.61	191.12	422.45	3072.55
Dirty	19.8	50.8	42.2	92.2	48.6	N/A	N/A	1.0	3	901.61	5.58	297.41	1810.58

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