PNNL-13434



# Verification of the Accuracy of Sample-Size Equation Calculations for Visual Sample Plan Version 0.9C

J. R. Davidson

January 2001



Prepared for the U.S. Department of Energy under Contract DE-AC06-76RL01830

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### **Summary**

Visual Sample Plan (VSP) is a software tool being developed to facilitate the design of environmental sampling plans using a site-map visual interface, standard equations for computing the number of samples (sample size) required for conducting statistical tests of hypotheses, a variety of sampling grids and random sampling plans, and graphs to visually depict the results to the user. The development of VSP has been ongoing for a number of years and several beta versions of the VSP code have been available for download from the web by individuals who wished to use a preliminary and partially tested code.

The VSP code has now been developed to a point where increased attention is being given to documenting that the calculations conducted by the code are accurate and contain no errors. This report documents the comparisons made in 1999 between the number of samples calculated by VSP Version 0.9C and the number of samples calculated by a computer code written in the S-PLUS<sup>®</sup> language.

The results of this report indicate that the sample-size equations used by version 0.9C of VSP to determine the recommended minimum number of sampling locations are properly implemented for the particular VSP inputs used. However, evaluations of version 0.9H of the VSP code, which were conducted after the evaluations of version 0.9C reported here, indicated that a revision of the sample-size equations was needed for three of the nine statistical tests in VSP; namely, the two-sample t test, the one-sample test of proportions, and the two-sample test of proportion. These evaluations of version 0.9H, which are reported in Gilbert et al (2001), indicated that the sample sizes computed for these three tests were in error for certain VSP input options not considered in the evaluations reported here for version 0.9C. These errors in VSP were corrected and will carry over to later versions.

This report also documents that the VSP implementation of the ELIPGRID-PC algorithm for hot spot probabilities matches previous results for 100 standard test cases. The Conclusions and Limitations section of this document lists some aspects of VSP that were not tested by this suite of tests and recommends simulation-based enhancements for future versions of VSP.

<sup>&</sup>lt;sup>®</sup> S-PLUS is a registered trademark of MathSoft, Inc., Cambridge, Massachusetts.

# Acknowledgments

John Wilson of Oak Ridge National Laboratory is the co-developer of VSP. VSP would either not exist or be much behind its present stage of development without John's rapid coding skills and invaluable ability to produce nearly bug-free code.

The author also acknowledges the vision of two managers who have been very supportive of the development of VSP - Brent Pulsipher, manager of Statistics Resources at Pacific Northwest National Laboratory, and Craig Little, manager of the Environmental Technology Section for Oak Ridge National Laboratory. It is also a pleasure to acknowledge Richard Gilbert and Brent Pulsipher for their thoughtful review and revision of this report.

The original algorithm used in Visual Sample Plan for hot-spot probability calculations was published in 1969 by Frans Wickman and Donald Singer, both then with Pennsylvania State University (Singer and Wickman 1969). In 1972, Singer published a computer code, ELIPGRID, to automate hot-spot probability calculations (Singer 1972). In 1987, Richard Gilbert of the Pacific Northwest National Laboratory (PNNL) published a statistical methods reference that included examples of calculating the probability of locating hot spots using ELIPGRID-based nomographs (Gilbert 1987). In 1995, Jim Davidson, at that time with Oak Ridge National Laboratory (ORNL), published ELIPGRID-PC, an upgraded and corrected version of the original ELIPGRID algorithm (Davidson 1995b). This program became the conceptual starting point for Visual Sample Plan. In 1997, John Wilson of ORNL began working with Jim on a Windows<sup>®</sup> 95 version of the program, which included many other sampling designs and a site-map user interface. In 1998, the web-based SampTOOL flowchart expert being developed by Richard Gilbert, Tim Schiebe, and Nancy Hassig, all with PNNL, began to be integrated into VSP in a limited way.

Other individuals have helped in developing of ELIPGRID-PC, VSP, and SampTOOL by providing conceptual ideas, constructive criticism, debugging support, graphics support, editorial support, logistics support, and encouragement. These individuals include Rick Bates, Rick Blancq, Mary Cliff, Phil Egidi, Nancy Hassig, Joella Krall, Al Laase, Bob O'Brien, Brenda Odom, Penny Roundtree, Sebastian Tindall, and Luci Walker.

<sup>&</sup>lt;sup>®</sup> Windows is a registered trademark of the Microsoft Corporation, Redmond, Washington.

### Nomenclature

The following symbols, listed in alphabetical order, are used in many of the sample-size equations. Other symbols that are used in only a few places are defined in the text near their first use.

- $\alpha$  is the probability of the statistical test making a Type I error, i.e., rejecting a true null hypothesis.
- $\beta$  is the probability of the statistical test making a Type II error, i.e., not rejecting a false null hypothesis.
- $\Delta$  is the width of the gray region, i.e., the distance from the Action Level to the outer bound of the gray region in the Decision Performance Goal Diagram used in Step 6 of the Data Quality Objectives process.
- *n* is the minimum recommended number of sampling locations at the study site.
- *m* is the minimum recommended number of sampling locations at a second study site, for example, a reference or background site.

$$\overline{x}$$
 is the arithmetic mean;  $\overline{x} = \frac{1}{n} \sum_{i=1}^{n} x_i$ .

*s* is the sample standard deviation; 
$$s = \sqrt{\frac{1}{(n-1)} \sum_{i=1}^{n} (x_i - \overline{x})^2}$$
.

 $\Phi$  is the cumulative standard normal distribution function;  $\Phi(z) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{z} e^{-\frac{1}{2}x^2} dx$ .

- $z_{1-\alpha}$  is the value of the standard normal distribution (the normal distribution with mean zero and standard deviation 1) for which  $100(1 \alpha)\%$  of the distribution is less than  $z_{1-\alpha}$
- $z_{1-\beta}$  is the value of the standard normal distribution for which  $100(1 \beta)\%$  of the distribution is less than  $z_{1-\beta}$ .
- $t_{1-\alpha, df}$  is the value of the student's *t*-distribution with *df* degrees of freedom for which  $100(1 \alpha)\%$  of the distribution is less than  $t_{1-\alpha, df}$ . The degrees of freedom are *n* 1 in VSP unless otherwise specified.

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# **1.0 Introduction**

Visual Sample Plan (VSP) is a software tool developed to facilitate the design of environmental sampling plans using a site-map visual interface, standard equations for computing the number of samples (sample size) required for a suite of statistical hypothesis tests, a variety of sampling grids and random sampling plans, and graphs to visually depict the results to the user. VSP also can be used retrospectively to decide if a completed sampling design employed enough samples to make a desired hypothesis test statistically significant at specified decision error rates. Thus, VSP can assist the team planning an environmental sampling design at the beginning of a project as well as in assessing a survey after it has been completed.

Currently, VSP provides four methods to determine the *number* of samples to collect:

- equations developed for parametric statistics tests
- equations developed for nonparametric statistics tests
- algorithms for hot-spot-sampling problems
- judgment sampling, which allows the user to select the number of samples.

VSP provides five methods to determine sampling *locations*:

- simple random sampling (SRS)
- systematic grid sampling using square, triangular, or rectangular grids
- hot-spot sampling using square, triangular, or rectangular grids
- adaptive-fill sampling in which previous sampling locations are avoided in the selection of new locations
- manual selection in which the user picks the location by hand.

The VSP tool provides two types of random number generators for randomly selecting a sampling location:

- a pseudo-random number generator where each location has an equal and independent chance of being sampled
- a quasi-random number generator where locations chosen during the current sampling plan are avoided.

The purpose of this report is to document the results of sample-size calculations made using a code written in the S-PLUS language to verify that the VSP implementation of the sample-size equations for various statistical tests of hypotheses is correct. This report provides comparisons between the number of samples calculated by version 0.9C of VSP and the number of samples calculated by the S-PLUS code for specified VSP input options. The sample sizes calculated are presented in Appendix A. The S-PLUS code is provided in Appendix B.

It should be noted that the algorithms and random number generators used for selecting sampling *locations* are not within the scope of this document. Also, readers of this report are assumed to have a good understanding of the Data Quality Objectives Process and associated statistical concepts.

# 2.0 Simple Random Sampling Designs

Simple random sampling (SRS) is the most simple and fundamental probability-based method for selecting sampling locations. SRS designs imply that any sampling location is equally likely to be selected to be sampled and the selection of one sampling location does not influence the selection of other locations. See Gilbert (1987) for more information on SRS designs.

### 2.1 Sample Size Equations for Parametric Statistics Tests

The following parametric statistics tests are used in VSP:

- One-sample t test
- Two-sample t test

The equations VSP uses to compute the number of samples (sample-size) for the two t tests above are from EPA (1996).

In addition to the above tests, VSP also computes the number of samples required for calculating a confidence interval for a mean using the method in Gilbert (1987, p. 32). The two tests and the confidence interval are appropriate if the data obtained are normally distributed or if enough samples are collected such that the distribution of the computed mean of the collected data is normally distributed. If the data or the computed mean are not at least approximately normally distributed then one of the nonparametric tests in Section 3.0 should be considered for use.

It is noted that the selection of a statistical test of hypothesis is an important consideration because the equation used in VSP to compute the number of samples required depends in part on the particular test selected, which in turn depends on the probability distribution of the data. Currently, VSP does not explicitly take into account any information the VSP user may have on the data distribution that applies to the study site of interest. However, consideration is being given to enhancing VSP so that data distribution information for the study site may be used by VSP in a simulation routine to determine the number of samples for any selected test or tests in VSP that are being considered for use. If that enhancement is made, then the VSP user could select the test that requires the smallest number of samples that would achieve the statistical test performance goals in terms of the test making correct conclusions.

#### 2.1.1 Results for VSP Option Mean vs. Action Level: The One-Sample t - Test

The sample-size equation used for this option is (EPA 1996, p. 3.2-3)

$$n = \frac{(z_{1-\alpha} + z_{1-\beta})^2 s^2}{\Delta^2} + 0.5 z_{1-\alpha}^2$$
(1)

VSP's implementation of this equation was tested using the VSPTest program written in S-PLUS. This program generated 15 test cases using random numbers drawn from a uniform distribution for alpha ( $\alpha$ ), beta ( $\beta$ ), delta ( $\Delta$ ), and the standard deviation (s). The original test file is in Appendix A, and the S-PLUS code is in Appendix B. In VSP, the null hypothesis "true mean  $\geq$  action level" was selected and the test parameters for each test case in Table 2.1 were entered into the VSP "Mean vs. Action Level" dialog box. The VSP-calculated sample size is recorded in the "VSP-Calculated Sample Size" column in Table 2.1. All VSP-calculated sample-size values agree with the values calculated by the test code.

**Table 2.1**. Tests of VSP Option, Simple Random Sampling  $\rightarrow$  Parametric  $\rightarrow$  Mean vs. Action Level:<br/>One-Sample *t*-Test

Test Case	Alpha	Beta	Delta	Standard Deviation	Test-Code- Calculated Sample Size	VSP- Calculated Sample Size
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	0.16	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

#### 2.1.2 Results for VSP Option Mean vs. Reference Mean: The Two-Sample t-Test

The sample-size equation used for this option is (EPA 1996, pp. 3.3 to 3.5)

$$n = \frac{2(z_{1-\alpha} + z_{1-\beta})^2 s^2}{\Delta^2} + 0.25 z_{1-\alpha}^2$$
(2)

VSP's implementation of this equation was tested using the VSPTest program written in S-PLUS. This program generated 15 test cases using random numbers drawn from a uniform distribution for alpha, beta, delta, and the standard deviation. The original test file is in Appendix A, and the S-PLUS code is in Appendix B. In VSP, the null hypothesis "difference of the means ≥ specified difference" was selected and the test parameters for each test case in Table 2.2 were entered into the "Mean vs. Reference Area Mean" dialog box. The VSP-calculated sample size is recorded in the "VSP-Calculated Sample Size" column in Table 2.2. All VSP-calculated values agree with the values calculated by the test code.

**Table 2.2.** Tests of VSP Option, Simple Random Sampling  $\rightarrow$  Parametric  $\rightarrow$  Mean vs. Reference Area<br/>Mean: Two-Sample *t*-Test

				Standard	Test-Code- Calculated	VSP- Calculated
Test Case	Alpha	Beta	Delta	Deviation	Sample Size	Sample Size
1	0.22	0.22	4.43	3.20	3	3
2	0.06	0.08	3.52	2.66	11	11
3	0.19	0.16	1.19	4.52	102	102
4	0.14	0.13	0.38	2.55	439	439
5	0.07	0.18	0.25	4.28	3353	3353
6	0.12	0.24	2.79	0.86	2	2
7	0.03	0.03	3.02	3.87	48	48
8	0.10	0.21	1.99	7.17	114	114
9	0.05	0.15	3.75	9.87	101	101
10	0.14	0.14	0.94	5.33	301	301
11	0.23	0.24	4.66	6.54	9	9
12	0.23	0.21	4.15	3.16	3	3
13	0.02	0.17	3.79	9.62	118	118
14	0.02	0.16	3.13	6.69	86	86
15	0.14	0.09	3.75	9.21	72	72

#### 2.1.3 Results for VSP Option Confidence Interval for a Mean

The sample-size equation used for this option is from Gilbert (1987, p. 32):

$$n = \left[\frac{t_{1-\alpha,df}S}{d}\right]^2 \tag{3}$$

The *t*-distribution value is based on the degrees of freedom, df = n - 1. Equation (3) must be solved iteratively because *n* appears on both sides. VSP's implementation of this equation, was tested using the VSPTest program written in S-PLUS. This program generated 15 test cases using random numbers drawn from a uniform distribution for the confidence level, the standard deviation, and the desired half-width of the confidence interval. The original test file is in Appendix A, and the S-PLUS code is in Appendix B. The test results are found in Table 2.3. In VSP, the parameters for each test case in Table 2.3 were entered into the "VSP-Confidence Interval for a Mean" dialog box and the VSP-calculated sample size is recorded in the "VSP-Calculated Sample Size" column in Table 2.3. All VSP-calculated values agree with the values calculated by the test code.

Test Case	Туре	Confidence Level	Standard Deviation	Half-Width Confidence Interval	Test-Code- Calculated Sample Size	VSP- Calculated Sample Size
1	Two-Sided	0.93	8.90	0.64	637	637
2	One-Sided	0.60	7.13	0.53	13	13
3	Two-Sided	0.86	2.62	0.90	20	20
4	One-Sided	0.77	1.05	0.51	4	4
5	Two-Sided	0.63	0.79	0.86	2	2
6	Two-Sided	0.73	5.72	0.17	1379	1379
7	One-Sided	0.54	6.17	0.77	2	2
8	Two-Sided	0.69	4.17	1.43	10	10
9	Two-Sided	0.58	7.57	1.97	11	11
10	Two-Sided	0.76	2.13	1.07	7	7
11	Two-Sided	0.95	9.35	1.31	198	198
12	Two-Sided	0.94	8.35	0.63	623	623
13	Two-Sided	0.52	7.65	1.92	9	9
14	Two-Sided	0.53	6.38	1.34	13	13
15	One-Sided	0.77	7.57	1.84	11	11

<b>Table 2.3.</b> Tests of VSP Option, Simple Random Sampling $\rightarrow$ Parametric $\rightarrow$ Confidence Interval for a
Mean

### 2.2 Sample-Size Equations for Nonparametric Statistics Tests

VSP also permits the user to select a nonparametric statistical test of hypothesis.

The following nonparametric tests use sample-size equations found in *Guidance for Data Quality Assessment* (EPA 1996):

- Mean vs. Action Level: Wilcoxon Signed Rank Test
- Proportion vs. Given Proportion: One-Sample Proportion Test
- Comparison of Two Proportions: Two-Sample Proportion Test
- Comparison of Two Populations: Wilcoxon Rank Sum Test.

The following nonparametric tests use sample size equations found in the *Multi-Agency Radiation Survey* and Site Investigation Manual (MARSSIM) (EPA 1997):

MARSSIM Sign Test: Median vs. Action Level
MARSSIM WRS Test: Median vs. Background Level.

Please see the MARSSIM guidance document (EPA 1997, pp. 2-34 to 2-38) for a discussion of the advantages and disadvantages of nonparametric tests.

The sample-size equations used for the nonparametric and parametric statistical tests in VSP are commonly used to approximate the number of samples required for the statistical tests. However, a valuable future addition to VSP would be a simulation capability that would empirically compare the sample-size requirements of parametric and nonparametric tests for a given data distribution. That is, for a specific data distribution believed to be appropriate for a study site, VSP could be coded to empirically determine the number of samples required for appropriate parametric tests and their nonparametric competitors for that particular data distribution. For some distributions the nonparametric test may require fewer samples to achieve the required test performance than that needed by a parametric test. Or, the opposite could occur. A choice of which test to use for the situation at hand could be made on the basis of the number of samples required. Consideration is being given to incorporating this added capability in VSP.

#### 2.2.1 Results for VSP Option Mean vs. Action Level: Wilcoxon Signed Rank Test

The sample-size equation used for this option is (EPA 1996, p. 3.2-8)

$$n = 1.16 \times \left[ \frac{s^2 (z_{1-\alpha} + z_{1-\beta})^2}{\Delta^2} + 0.5 z_{1-\alpha}^2 \right]$$
(4)

VSP's implementation of this equation was tested using the VSPTest program written in S-PLUS. This program generated 15 test cases using random numbers drawn from a uniform distribution for alpha, beta, delta, and the standard deviation. The original test file is in Appendix A, and the S-PLUS code is in Appendix B. In VSP, the null hypothesis "true mean  $\geq$  action level" was selected and the test parameters for each test case in Table 2.4 were entered into the "Mean vs. Action Level Wilcoxon Signed Rank Test" dialog box. The VSP-calculated sample size is recorded in the "VSP Calculated Sample Size" column in Table 2.4. All VSP-calculated values agree with the values calculated by the S-PLUS test code.

Test Case	Alpha	Beta	Delta	Standard Deviation	Test-Code- Calculated Sample Size	VSP- Calculated Sample Size
1	0.22	0.22	4.43	3.20	2	2
2	0.06	0.08	3.52	2.66	8	8
3	0.19	0.16	1.19	4.52	60	60
4	0.14	0.13	0.38	2.55	256	256
5	0.07	0.18	0.25	4.28	1946	1946
6	0.12	0.24	2.79	0.86	2	2
7	0.03	0.03	3.02	3.87	30	30
8	0.10	0.21	1.99	7.17	67	67
9	0.05	0.15	3.75	9.87	60	60
10	0.14	0.14	0.94	5.33	175	175
11	0.23	0.24	4.66	6.54	6	6
12	0.23	0.21	4.15	3.16	2	2
13	0.02	0.17	3.79	9.62	71	71
14	0.02	0.16	3.13	6.69	52	52
15	0.14	0.09	3.75	9.21	42	42

**Table 2.4.** Tests of VSP Option, Simple Random Sampling  $\rightarrow$  Nonparametric  $\rightarrow$  Mean (or Median) vs. Action Level: Wilcoxon Signed Rank Test

#### 2.2.2 Results for VSP Option Proportion vs. Given Proportion: One-Sample Proportion Test

The sample-size equation used for this option is (EPA 1996, p. 3.2-12)

$$n = \left[\frac{z_{1-\alpha}\sqrt{P_0(1-P_0)} + z_{1-\beta}\sqrt{P_1(1-P_1)}}{P_1 - P_0}\right]^2$$
(5)

where  $P_0$  is the given proportion, i.e., the Action Level and  $P_1$  is the outer bound of the gray region.

VSP's implementation of this equation was tested using the VSPTest program written in S-PLUS. This program generated 15 test cases using random numbers drawn from a uniform distribution for alpha, beta, delta, and  $P_0$ . The original test file is in Appendix A, and the S-PLUS code is in Appendix B. The test results are found in Table 2.5. In VSP, the null hypothesis "True mean  $\geq$  action level" was selected and the test parameters were entered into the "Proportion vs. Given Proportion" dialog box. The VSP-calculated sample size is recorded in the "VSP-Calculated Sample Size" column in Table 2.5. All VSP-calculated values agree with the values calculated by the test code.

					Test-Code-	VSP-
					Calculated	Calculated
Test Case	Alpha	Beta	Delta	P <sub>0</sub>	Sample Size	Sample Size
1	0.22	0.22	0.289	0.29	2	2
2	0.06	0.08	0.229	0.23	10	10
3	0.19	0.16	0.120	0.43	56	56
4	0.14	0.13	0.040	0.22	485	48
5	0.07	0.18	0.020	0.40	3407	3407
6	0.12	0.24	0.049	0.05	33	33
7	0.03	0.03	0.300	0.36	21	21
8	0.10	0.21	0.200	0.70	25	25
9	0.05	0.15	0.370	0.98	4	4
10	0.14	0.14	0.090	0.51	143	143
11	0.23	0.24	0.460	0.63	2	2
12	0.23	0.21	0.279	0.28	2	2
13	0.02	0.17	0.370	0.95	7	7
14	0.02	0.16	0.310	0.65	22	22
15	0.14	0.09	0.370	0.91	7	7

**Table 2.5.** Tests of VSP Option, Simple Random Sampling  $\rightarrow$  Nonparametric  $\rightarrow$  Proportion vs. Given<br/>Proportion: One-Sample Proportion Test

# 2.2.3 Results for VSP Option Comparison of Two Proportions: Two-Sample Proportion Test

The sample-size equation used for this option is (EPA 1996, p. 3.3-8)

$$m = n = \frac{2(z_{1-\alpha} + z_{1-\beta})^2 \overline{P}(1-\overline{P})}{(P_1 - P_2)^2}$$
(6)

where

- n = the minimum sample size for the survey unit
- m = the minimum sample size for the reference area
- $P_1$  = the unknown proportion in the survey unit. VSP estimates  $P_1$  using  $P_1 = P_2 \pm \Delta$  and chooses  $P_1$  so that  $\overline{P}$  is closest to 0.5
- $P_2$  = the estimated proportion in the reference area entered by the user
- $\overline{P}$  = the average proportion,  $(P_1 + P_2)/2$
- $\Delta$  = the minimum difference in proportions to be detected at the given error rates (for this version  $\Delta > 0$  and  $\Delta \le 0.5$ ).

VSP's implementation of this equation was tested using the VSPTest program written in S-PLUS. This program generated 15 test cases using random numbers drawn from a uniform distribution for alpha, beta, delta,  $P_1$  and  $P_2$ . The original test file is in Appendix A, and the S-PLUS code is in Appendix B. The test results are found in Table 2.6. In VSP, the null hypothesis "difference in proportions  $\geq$  specified difference" was selected and the test parameters were entered into the "Comparison of Two Proportions"

dialog box. The VSP-calculated sample size is recorded in the "VSP-Calculated Sample Size" column in Table 2.6. All VSP-calculated values agree with the values calculated by the S-PLUS test code.

Test Case	Alpha	Beta	Delta	P <sub>1</sub>	P <sub>2</sub>	Test-Code- Calculated Sample Size	VSP- Calculated Sample Size
1	0.22	0.22	0.44	0.72	0.28	7	7
2	0.06	0.08	0.35	0.57	0.22	35	35
3	0.19	0.16	0.12	0.54	0.42	122	122
4	0.14	0.13	0.04	0.25	0.21	1079	1079
5	0.07	0.18	0.03	0.42	0.39	3062	3062
6	0.12	0.24	0.28	0.32	0.04	14	14
7	0.03	0.03	0.30	0.65	0.35	79	79
8	0.10	0.21	0.20	0.49	0.69	53	53
9	0.05	0.15	0.37	0.61	0.98	18	18
10	0.14	0.14	0.09	0.59	0.50	286	286
11	0.23	0.24	0.47	0.16	0.63	5	5
12	0.23	0.21	0.41	0.69	0.28	8	8
13	0.02	0.17	0.38	0.57	0.95	23	23
14	0.02	0.16	0.31	0.34	0.65	49	49
15	0.14	0.09	0.37	0.54	0.91	18	18

**Table 2.6**. Tests of VSP Option, Simple Random Sampling  $\rightarrow$  Nonparametric  $\rightarrow$  Comparison of Two<br/>Proportions: Two-Sample Proportion Test

#### 2.2.4 Test Results for VSP Option Comparison of Two Populations: Wilcoxon Rank Sum Test

The sample-size equation used for this option is (EPA 1996, pp. 3.3-10 to 3.3-12)

$$m = n = 1.16 \times \left[ \frac{2s^2 (z_{1-\alpha} + z_{1-\beta})^2}{\Delta^2} + 0.25 z_{1-\alpha}^2 \right]$$
(7)

where

n = the minimum sample size for the survey unit

- m = the minimum sample size for the reference area
- $\Delta$  = the width of the gray region, i.e., the minimum difference between the two means detectable at the given error rates.

[Note that EPA (1996) defines m to be the sample size for the survey unit and n to be the sample size for the reference area.]

VSP's implementation of this equation was tested using the VSPTest program written in S-PLUS. This program generated 15 test cases using random numbers drawn from a uniform distribution for alpha, beta, delta, and the standard deviation. The original test file is in Appendix A, and the S-PLUS code is in Appendix B. The test results are found in Table 2.7. In VSP, the null hypothesis "difference of the

means  $\geq$  specified difference" was selected and the test parameters were entered into the "Comparison of Two Populations" dialog box. The VSP-calculated sample size is recorded in the "VSP-Calculated Sample Size" column in Table 2.7. All VSP-calculated values agree with the values calculated by the test code.

				Standard	Test-Code- Calculated	VSP- Calculated
Test Case	Alpha	Beta	Delta	Deviation	Sample Size	Sample Size
1	0.22	0.22	4.43	3.20	4	4
2	0.06	0.08	3.52	2.66	13	13
3	0.19	0.16	1.19	4.52	118	118
4	0.14	0.13	0.38	2.55	510	510
5	0.07	0.18	0.25	4.28	3889	3889
6	0.12	0.24	2.79	0.86	2	2
7	0.03	0.03	3.02	3.87	55	55
8	0.10	0.21	1.99	7.17	132	132
9	0.05	0.15	3.75	9.87	117	117
10	0.14	0.14	0.94	5.33	349	349
11	0.23	0.24	4.66	6.54	10	10
12	0.23	0.21	4.15	3.16	4	4
13	0.02	0.17	3.79	9.62	137	137
14	0.02	0.16	3.13	6.69	100	100
15	0.14	0.09	3.75	9.21	83	83

**Table 2.7**. Tests of VSP Option, Simple Random Sampling → Nonparametric → Comparison of Two Populations: QA/G-9 Wilcoxon Rank Sum Test

#### 2.2.5 Results for VSP Option MARSSIM Sign Test: Median vs. Action Level

The sample-size equation used for this option is (EPA 1997, p. 5-33)

$$n = \frac{(z_{1-\alpha} + z_{1-\beta})^2}{4(SignP - 0.5)^2}$$
(8)

where SignP is calculated using (Gogolak, Powers, and Huffert 1997, p. 9-3)

$$SignP = \Phi\left(\frac{\Delta}{\sigma}\right) \tag{9}$$

VSP's implementation of this equation was tested using the VSPTest program written in S-PLUS. This program generated 15 test cases using random numbers drawn from a uniform distribution for alpha, beta, delta, the standard deviation, and *SignP*. The original test file is in Appendix A, and the S-PLUS code is in Appendix B. The test results are found in Table 2.8. In VSP, the null hypothesis "true median  $\geq$  action level" was selected and the parameters were entered into the "MARSSIM Sign Test" dialog box. The VSP-calculated sample size is recorded in the "VSP-Calculated Sample Size" column in Table 2.8. All VSP-calculated values agree with the values calculated by the test code.

Test Case	Alpha	Beta	Delta	Standard Deviation	SignP	Test-Code- Calculated Sample Size	VSP- Calculated Sample Size
1	0.22	0.22	4.43	3.20	0.917	4	4
2	0.06	0.08	3.52	2.66	0.907	14	14
3	0.19	0.16	1.19	4.52	0.604	82	82
4	0.14	0.13	0.38	2.55	0.559	348	348
5	0.07	0.18	0.25	4.28	0.523	2636	2636
6	0.12	0.24	2.79	0.86	0.999	4	4
7	0.03	0.03	3.02	3.87	0.782	45	45
8	0.10	0.21	1.99	7.17	0.609	92	92
9	0.05	0.15	3.75	9.87	0.648	83	83
10	0.14	0.14	0.94	5.33	0.570	239	239
11	0.23	0.24	4.66	6.54	0.762	8	8
12	0.23	0.21	4.15	3.16	0.905	4	4
13	0.02	0.17	3.79	9.62	0.653	97	97
14	0.02	0.16	3.13	6.69	0.680	72	72
15	0.14	0.09	3.75	9.21	0.658	59	59

**Table 2.8**. Tests of VSP Option, Simple Random Sampling  $\rightarrow$  Nonparametric  $\rightarrow$  MARSSIM Sign Test:Median vs. Action Level

#### 2.2.6 Results for VSP Option MARSSIM WRS Test: Median vs. Background Level

The sample-size equation used for this option is (EPA 1997, p. 5-28)

$$n = \frac{(z_{1-\alpha} + z_{1-\beta})^2}{3(P_r - 0.5)^2}$$
(10)

where *n* is the minimum number of samples for a survey unit *and* the reference area and  $P_r$  is calculated using (Gogolak, Powers, and Huffert 1997, p. 9-11)

$$P_r = \Phi\left(\frac{\Delta}{\sqrt{2}\sigma}\right) \tag{11}$$

VSP's implementation of this equation was tested using the VSPTest program written in S-PLUS. This program generated 15 test cases using random numbers drawn from a uniform distribution for alpha, beta, delta, the standard deviation, and  $P_r$ . The original test file is in Appendix A, and the S-PLUS code is in Appendix B. The test results are found in Table 2.9. In VSP, the null hypothesis "true median  $\geq$  action level was selected and the test parameters were entered into the "MARSSIM WRS Test" dialog box. The VSP-calculated sample size is recorded in the "VSP-Calculated Sample Size" column in Table 2.9. All VSP-calculated values agree with the values calculated by the test code.

Test Case	Alpha	Beta	Delta	Standard Deviation	Pr	Test-Code- Calculated Sample Size	VSP- Calculated Sample Size
1	0.22	0.22	4.43	3.20	0.836	4	4
2	0.06	0.08	3.52	2.66	0.825	14	14
3	0.19	0.16	1.19	4.52	0.574	108	108
4	0.14	0.13	0.38	2.55	0.542	461	461
5	0.07	0.18	0.25	4.28	0.516	3512	3512
6	0.12	0.24	2.79	0.86	0.989	3	3
7	0.03	0.03	3.02	3.87	0.709	54	54
8	0.10	0.21	1.99	7.17	0.578	121	121
9	0.05	0.15	3.75	9.87	0.606	107	107
10	0.14	0.14	0.94	5.33	0.550	316	316
11	0.23	0.24	4.66	6.54	0.693	10	10
12	0.23	0.21	4.15	3.16	0.823	4	4
13	0.02	0.17	3.79	9.62	0.610	126	126
14	0.02	0.16	3.13	6.69	0.630	93	93
15	0.14	0.09	3.75	9.21	0.613	77	77

**Table 2.9**. Tests of VSP Option, Simple Random Sampling  $\rightarrow$  Nonparametric  $\rightarrow$  MARSSIM WRS Test:Median vs. Background Level

### 2.3 Predetermined Number of Samples

The VSP option, Simple Random Sampling  $\rightarrow$  Predetermined, allows the user to enter an arbitrary sample size. This allows the user to enter the number of samples required for a sampling design not currently supported by VSP. Because the user independently determines the sample size, there is no sample size equation to test for this option.

# 3.0 Other Sampling Designs

### 3.1 Parametric and Nonparametric Tests and Systematic Grid Sampling

The Systematic Grid Sampling  $\rightarrow$  Parametric options and the Systematic Grid Sampling  $\rightarrow$ Nonparametric options all use the sample-size equations listed in Section 2. The difference is in the way the sample locations are determined. For systematic-grid sampling, only the first point is selected at random. The remaining points are chosen from a square, triangular, or rectangular grid pattern starting at the randomly selected location. In some cases, the recommended minimum number of samples may be slightly higher for the grid sampling designs than the random sampling designs. This is due to the need for completing the balanced aspects required for grids.

### **3.2** Locating Hot Spots

As modifications are made to the ELIPGRID-PC algorithm, it is important to demonstrate the continuing integrity of the core algorithm. Singer gave 100 test cases divided between square, rectangular, and triangular grids that provide a test suite to check new ELIPGRID versions (Singer 1972). These 100 cases in corrected order as described by Davidson (1994, Table B.1) can be found in file Test100.Sif listed in Appendix C. The output for these test cases using the VSP implementation of the ELIPGRID-PC algorithm can be found in file Test100.Out listed in Appendix D. All VSP-calculated results listed in file Test100.Out match the ELIPGRID-PC results found in file Test100.Out listed in Table B.2 (Davidson 1995b).

The Systematic Grid Sampling  $\rightarrow$  Locating Hot Spots options that depend on numerical search routines to find grid sizes or hot-spot sizes for specified conditions have not been independently tested. Internal cross-comparisons between these options and comparisons with externally calculated results would be helpful. However, this goes beyond the scope of the current test suite.

### 3.3 Judgment Sampling

VSP allows the user to manually add any number of sampling locations at any location in a highlighted survey unit. Because the number and location of the samples are arbitrary, there is no sample-size equation to test for this option.

# 4.0 Conclusions and Limitations

The comparisons given above between VSP-calculated sample sizes and sample sizes calculated by the S-PLUS test code verify that the sample-size equations used by version 0.9C of VSP are properly implemented for the set of VSP input options and scenarios used. However, all testing conducted in 1999 and reported here was for the case where the null hypothesis was "site does not meet the standard" (the specific wording of this generic null hypothesis varies for the different tests). Tests of version 0.9H of VSP reported in Gilbert et al (2001) indicated that the sample sizes for the one-sample test of proportion were not correctly computed when the null hypothesis "site does meet the standard" was selected by the VSP user. Also, it was determined that modifications to the two-sample test of proportion and the two-sample t test were also required. Hence, the results in both this report and the Gilbert et al (2001) report must be used together to get a clear picture of the testing efforts made to verify that version 0.9H of VSP is correctly computing sample sizes.

Several other limitations in the testing done for this report should be noted.

- The VSP implementation of the hot-spot options that use numerical search algorithms were not validated. A full validation of these options would probably require some type of simulation approach such as used by Davidson (1995a). That level of effort is beyond the scope of this document.
- The adaptive-fill option and the quasi-random sampling options were not tested. Testing these two options was beyond the scope of this document.
- The Measurement Quality Objectives (MQO) module of VSP version 0.9H was not tested because that model was not implemented in the version 0.9C tested here.

Finally, it should be noted that version 0.9C of VSP uses only equations to find recommended sample sizes. While this is the method that is widely used, it is recommended that computer simulation techniques be utilized in future versions as an adjunct to the equation-based methods currently used. Determining how many samples to take for an environmental sampling problem should make use of the powerful computing capabilities widely available through inexpensive PC technology.

### 5.0 References

Conover WJ. 1980. Practical nonparametric statistics. John Wiley & Sons, New York.

Davidson JR. 1994. *ELIPGRID-PC: a program for calculating hot spot probabilities*. ORNL/TM-12774, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Davidson JR. 1995a. *Monte Carlo tests of the ELIPGRID-PC algorithm*. ORNL/TM-12774, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Davidson, JR. 1995b. *ELIPGRID-PC: upgraded version*. ORNL/TM-13103, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

EPA. 1996. *Guidance for data quality assessment*. EPA QA/G-9, EPA/600/R-96084, Office of Research and Development, Quality Assurance Division, U.S. Environmental Protection Agency, Washington, D.C.

EPA. 1997. *Multi-agency radiation survey and site investigation manual (MARSSIM)*. EPA 402-R-97-016, NUREG-1575, U.S. Environmental Protection Agency, Washington, D.C.

Gilbert, RO. 1987. *Statistical methods for environmental pollution monitoring*. John Wiley & Sons, New York.

Gogolak CV, GE Powers, and AM Huffert. 1997. *A nonparametric statistical methodology for the design and analysis of final status decommissioning surveys*. NUREG-1505, U.S. Nuclear Regulatory Commission, Washington, D.C.

Hahn GJ, and SS Shapiro. 1967. Statistical models in engineering. John Wiley & Sons, New York.

Singer DA, and FE Wickman. 1969. *Probability tables for locating elliptical targets with square, rectangular and hexagonal point nets*. Pennsylvania State University, University Park, Pennsylvania.

Singer DA. 1972. "ELIPGRID, a FORTRAN IV Program for Calculating the Probability of Success in Locating Elliptical Targets with Square, Rectangular, and Hexagonal Grids." *Geocom Programs*, 4:1-19.

Appendix A Sample Sizes Calculated with S-PLUS Test Code

# Appendix A Sample Sizes Calculated with S-PLUS Test Code

This appendix contains the sample-size test file generated by the VSPTest program. Note that the "XXXX" values below are placeholders for VSP-calculated sample sizes.

File: Purpose: Date cre Test cod Version	P eated: M	on Jun 21 im Davids	dependent 12:21:44 on, PNNL	1999 Statistic		? algorithms
Tests of	Mean vs.	Action L	evel: One	-Sample t	-Test Eq	quation
Case	Alpha	Beta	Delta	StdDev.	Test n	VSP n
1,	0.22,	0.22,	4.43,	3.20,	2,	XXXX
2,	0.06,	0.08,	3.52,	2.66,	7,	XXXX
З,	0.19,	0.16,	1.19,	4.52,	51,	XXXX
4,	0.14,	0.13,	0.38,	2.55,	220,	XXXX
5,	0.07,	0.18,	0.25,	4.28,	1677,	XXXX
6,	0.12,	0.24,	2.79,	0.86,	2,	XXXX
7,	0.03,	0.03,	3.02,	3.87,	26,	XXXX
8,	0.10,	0.21,	1.99,	7.17,	58,	XXXX
9,	0.05,	0.15,	3.75,	9.87,	52,	XXXX
10,	0.14,	0.14,	0.94,	5.33,	151,	XXXX
11,	0.23,	0.24,	4.66,	6.54,	5,	XXXX
12,	0.23,	0.21,		3.16,	2,	XXXX
13,	0.02,	0.17,		9.62,	61,	XXXX
14,	0.02,	0.16,	3.13,	6.69,	45,	XXXX
15,	0.14,	0.09,	3.75,	9.21,	36,	XXXX
Tests of	Mean vs.	Referenc	e Mean: I	wo-Sample	t-Test	Equation
Case	Alpha	Beta		StdDev.	Test n	VSP n
1,	0.22,	0.22,	4.43,	3.20,	З,	XXXX
2,	0.06,	0.08,	3.52,	2.66,	11,	XXXX
З,	0.19,	0.16,	1.19,	4.52,	102,	XXXX
4,	0.14,	0.13,	0.38,	2.55,	439,	XXXX
5,	0.07,	0.18,	0.25,	4.28,	3353,	XXXX
6,	0.12,	0.24,	2.79,	0.86,	2,	XXXX
7,	0.03,	0.03,	3.02,	3.87,	48,	XXXX
8,	0.10,	0.21,	1.99,	7.17,	114,	XXXX
9,	0.05,	0.15,	3.75,	9.87,	101,	XXXX
10,	0.14,	0.14,	0.94,	5.33,	301,	XXXX
11,	0.23,	0.24,		6.54,	9,	XXXX
12,	0.23,	0.21,	4.15,	3.16,	З,	XXXX
13,	0.02,	0.17,	3.79,	9.62,	118,	XXXX
14,	0.02,	0.16,		6.69,	86,	XXXX
15,	0.14,	0.09,	3.75,	9.21,	72,	XXXX

Tests of	Confidence In	terval for	a Mean			
Case	Type Conf	. Level	StdDev.	1/2 Widt	h Test n	VSP n
1,	Two-Sided,	0.93,	8.90,	0.64,	637,	XXXX
2,	One-Sided,	0.60,	7.13,	0.53,	13,	XXXX
З,	Two-Sided,	0.86,	2.62,	0.90,	20,	XXXX
4,	One-Sided,	0.77,	1.05,	0.51,	4,	XXXX
5,	Two-Sided,	0.63,	0.79,	0.86,	2,	XXXX
б,	Two-Sided,	0.73,	5.72,	0.17,	1379,	XXXX
7,	One-Sided,	0.54,	6.17,	0.77,	2,	XXXX
8,	Two-Sided,	0.69,	4.17,	1.43,	10,	XXXX
9,	Two-Sided,	0.58,	7.57,	1.97,	11,	XXXX
10,	Two-Sided,	0.76,	2.13,	1.07,	7,	XXXX
11,	Two-Sided,	0.95,	9.35,	1.31,	198,	XXXX
12,	Two-Sided,	0.94,	8.35,	0.63,	623,	XXXX
13,	Two-Sided,	0.52,	7.65,	1.92,	9,	XXXX
14,	Two-Sided,	0.53,	6.38,	1.34,	13,	XXXX
15,	One-Sided,	0.77,	7.57,	1.84,	11,	XXXX

Tests of Mean (or Median) vs. Action Level: Wilcoxon Signed Rank Test Equation

Case	Alpha	Beta	Delta	StdDev.	Test n	VSP n
1,	0.22,	0.22,	4.43,	3.20,	2,	XXXX
2,	0.06,	0.08,	3.52,	2.66,	8,	XXXX
З,	0.19,	0.16,	1.19,	4.52,	60,	XXXX
4,	0.14,	0.13,	0.38,	2.55,	256,	XXXX
5,	0.07,	0.18,	0.25,	4.28,	1946,	XXXX
6,	0.12,	0.24,	2.79,	0.86,	2,	XXXX
7,	0.03,	0.03,	3.02,	3.87,	30,	XXXX
8,	0.10,	0.21,	1.99,	7.17,	67,	XXXX
9,	0.05,	0.15,	3.75,	9.87,	60,	XXXX
10,	0.14,	0.14,	0.94,	5.33,	175,	XXXX
11,	0.23,	0.24,	4.66,	6.54,	6,	XXXX
12,	0.23,	0.21,	4.15,	3.16,	2,	XXXX
13,	0.02,	0.17,	3.79,	9.62,	71,	XXXX
14,	0.02,	0.16,	3.13,	6.69,	52,	XXXX
15,	0.14,	0.09,	3.75,	9.21,	42,	XXXX

Tests of	Proport	ion vs. G	iven Propo	rtion: One-	Sample Pr	oportio	n Test
Case	Alpha	Beta	Delta	PO	Test n	VSP n	
1,	0.22,	0.22,	0.289,	0.29,	2,	XXXX	
2,	0.06,	0.08,	0.229,	0.23,	10,	XXXX	
З,	0.19,	0.16,	0.120,	0.43,	56,	XXXX	
4,	0.14,	0.13,	0.040,	0.22,	485,	XXXX	
5,	0.07,	0.18,	0.020,	0.40,	3407,	XXXX	
6,	0.12,	0.24,	0.049,	0.05,	33,	XXXX	
7,	0.03,	0.03,	0.300,	0.36,	21,	XXXX	
8,	0.10,	0.21,	0.200,	0.70,	25,	XXXX	
9,	0.05,	0.15,	0.370,	0.98,	4,	XXXX	
10,	0.14,	0.14,	0.090,	0.51,	143,	XXXX	
11,	0.23,	0.24,	0.460,	0.63,	2,	XXXX	
12,	0.23,	0.21,	0.279,	0.28,	2,	XXXX	
13,	0.02,	0.17,	0.370,	0.95,	7,	XXXX	
14,	0.02,	0.16,	0.310,	0.65,	22,	XXXX	
15,	0.14,	0.09,	0.370,	0.91,	7,	XXXX	
Tests of	Two Pro	portions:	Two-Sample	e Test for 1	Proportio	ns	
Case	Alpha	Beta	Delta	P1 P2	2 T	est n	VSP n

1,	0.22,	0.22,	0.44,	0.72,	0.28,	7,	XXXX
2,	0.06,		0.35,	0.57,	0.22,	35,	XXXX
3,	0.19,		0.12,	0.54,	0.42,	122,	XXXX
	•						
4,	0.14,	0.13,	0.04,	0.25,	0.21,	1079,	XXXX
5,	0.07,	0.18,	0.03,	0.42,	0.39,	3062,	XXXX
6,	0.12,	0.24,	0.28,	0.32,	0.04,	14,	XXXX
7,	0.03,	0.03,	0.30,	0.65,	0.35,	79 <b>,</b>	XXXX
8,	0.10,	0.21,	0.20,	0.49,	0.69,	53,	XXXX
9,			0.37,	0.61,		18,	XXXX
10,			0.09,	0.59,	0.50,	286,	XXXX
11,	0.23,		0.47,	0.16,	0.63,	5,	XXXX
12,	0.23,	0.21,	0.41,	0.69,	0.28,	8,	XXXX
13,	0.02,	0.17,	0.38,	0.57,	0.95,	23,	XXXX
14,	0.02,	0.16,	0.31,	0.34,	0.65,	49,	XXXX
15,	0.14,	0.09,	0.37,	0.54,	0.91,	18,	XXXX
Tests	of Two Por	oulations:	OA/G-9	Wilcoxon Ra	ank Sum I	'est	
Case			Delta			VSP n	
1,			4.43,		4,	XXXX	
2,	0.06,	0.08,	3.52,		13,	XXXX	
3,	0.19,	0.16,	1.19,	4.52,	118,	XXXX	
4,	0.14,	0.13,	0.38,	2.55,	510,	XXXX	
5,	0.07,	0.18,	0.25,	4.28,	3889,	XXXX	
6,	0.12,	0.24,	2.79,	0.86,	2,	XXXX	
7,	0.03,	0.03,	3.02,	3.87,	55,	XXXX	
8,	0.10,		1.99,	7.17,	132,	XXXX	
9,			3.75,	9.87,	117,	XXXX	
10,			0.94,	5.33,	349,	XXXX	
10, 11,			4.66,	6.54,			
	0.23,	0.24,	4.00,		10,	XXXX	
12,	0.23,		4.15,	3.16,	4,	XXXX	
13,	0.02,	0.17,	3.79,		137,	XXXX	
14,	0.02,	0.16,	3.13,		100,	XXXX	
15,	0.14,	0.09,	3.75,	9.21,	83,	XXXX	
Tests	of MARSSIN	1 Sign Tes	t: Compa	arison of Me	edian vs.	Action Lev	vel
Case	Alpha	-	-	StdDev.			
1,	0.22,		4.43,			4,	XXXX
					0.907,		
2,	0.06,		3.52,			14,	XXXX
3,	0.19,	0.16,	1.19,	4.52,	0.604,	82,	XXXX
4,				2.55,		348,	XXXX
5,	0.07,	0.18,	0.25,	4.28,	0.523,	2636,	XXXX
6,	0.12,		2.79,		0.999,		XXXX
7,	0.03,	0.03,	3.02,	3.87,	0.782,	45,	XXXX
8,	0.10,	0.21,	1.99,	7.17,	0.609,	92,	XXXX
9,			3.75,		0.648,	83,	XXXX
10,			0.94,		570,	239,	XXXX
11,	0.23,				0.762,	8,	XXXX
					0.002,	3, 4,	
12,	0.23,	0.21,	4.15, 2.72	3.16,	0.905,		XXXX
13,	0.02,	0.17,	3.19,	9.62, 6.69,	0.653,	97,	XXXX
14,	0.02,	0.17,	3.13,	6.69,	0.680,	72,	XXXX
15,	0.14,	0.09,	3.75,	9.21,	0.658,	59,	XXXX
Tests	of MARSSIN	1 WRS Test	: Compai	rison of Med	lian vs.	Background	Level
Case	Alpha		Delta			Test r	
1,			4.43,			4,	
2,						14,	
		0.00,	1 10	2.66,	0.020,		XXXX
З,	0.19,	0.16,	±.19,	4.52,	0.5/4,	108,	XXXX

4,	0.14,	0.13,	0.38,	2.55,	0.542,	461,	XXXX
5,	0.07,	0.18,	0.25,	4.28,	0.516,	3512,	XXXX
б,	0.12,	0.24,	2.79,	0.86,	0.989,	3,	XXXX
7,	0.03,	0.03,	3.02,	3.87,	0.709,	54,	XXXX
8,	0.10,	0.21,	1.99,	7.17,	0.578,	121,	XXXX
9,	0.05,	0.15,	3.75,	9.87,	0.606,	107,	XXXX
10,	0.14,	0.14,	0.94,	5.33,	0.550,	316,	XXXX
11,	0.23,	0.24,	4.66,	6.54,	0.693,	10,	XXXX
12,	0.23,	0.21,	4.15,	3.16,	0.823,	4,	XXXX
13,	0.02,	0.17,	3.79,	9.62,	0.610,	126,	XXXX
14,	0.02,	0.16,	3.13,	6.69,	0.630,	93,	XXXX
15,	0.14,	0.09,	3.75,	9.21,	0.613,	77,	XXXX
End run:	VSPTest						

Appendix B S-PLUS Test Code

# Appendix B S-PLUS Test Code

The following code was written for S-PLUS 4.5 Professional Release 1 and run under the Microsoft<sup>®</sup> Windows<sup>®</sup> 95 operating system.

```
"VSPTest" <- function(NumCases=15,
   OutFile="VSPTest.Txt",
   Version="VSP 0.9C 06/02/99 1:09 PM")
# Function: VSPTest
# Purpose.: Provides independent tests of selected VSP algorithms
# Usage...: VSPTest() provides the default, NumCases, test cases
# Started.: 06/04/99
# Last Mod: 06/21/99
# Author..: Jim Davidson, PNNL Statistics Group
# Modifications:
# 06/21/99 Corrected spelling error
# 06/16/99 Modified MARSSIM WRS code to match VSP method of rounding
# 06/10/99 Final modifications to code before running test file
#______
cat("Running VSPTest...\n")
cat("Output file:", OutFile,"\n")
sink(OutFile)
cat("File:
                  ",OutFile,"\n")
cat("Purpose:
                  Provide independent tests of the VSP algorithms\n")
cat("Date created: ",date(),"\n")
cat("Test code by: Jim Davidson, PNNL Statistics Group\n")
cat("Version tested:",Version,"\n")
#---- Tests of Mean vs. Action Level: One-Sample t-Test Equation ----
cat("\nTests of Mean vs. Action Level: One-Sample t-Test Equation\n")
cat("Case Alpha Beta Delta StdDev. Test n VSP n\n")
# Force the same string of "random" numbers each time
set.seed(4)
# Generate NumCases random test cases
for(i in 1:NumCases) {
   Alpha <- round(runif(1, .01, .25), digits=2)
            <- round(runif(1, .01, .25), digits=2)
   Beta
  Delta <- round(runif(1, .1, 5.0), digits=2)
   StdDev
           <- round(runif(1, 0.5, 10.0), digits=2)
   Z1MinusA <- qnorm(1.0 - Alpha)
   Z1MinusB <- gnorm(1.0 - Beta)
   # Calculate sample size using EPA 1996, p. 3.2-3
  NumSamples
              <- ceiling(((Z1MinusA + Z1MinusB)*StdDev/Delta)<sup>2</sup> +
      0.5*Z1MinusA<sup>2</sup>)
   # Put numbers in correct format
   cat(paste(
               PadL(i,2),
               PadR(Alpha,4,"0"),
               PadR(Beta, 4, "0"),
               PadR(Delta,4,"0"),
               PadR(StdDev,4,"0"),
               PadL(NumSamples,4),"XXXX",sep=",\t\t"),"\n")
}
#---- Tests of Mean vs. Reference Mean: Two-Sample t-Test Equation ----
cat("\nTests of Mean vs. Reference Mean: Two-Sample t-Test Equation\n")
cat("Case Alpha Beta Delta StdDev. Test n VSP n\n")
```

# Force the same string of "random" numbers each time

```
set.seed(4)
# Generate NumCases random test cases
for(i in 1:NumCases) {
   Alpha
             <- round(runif(1, .01, .25), digits=2)
             <- round(runif(1, .01, .25), digits=2)
   Beta
   Delta <- round(runif(1, .1, 5.0), digits=2)</pre>
   StdDev <- round(runif(1, 0.5, 10.0), digits=2)</pre>
   Z1MinusA <- qnorm(1.0 - Alpha)
   Z1MinusB <- qnorm(1.0 - Beta)
   # Calculate sample size EPA 1996, pp. 3.3-3 to 3.3-5
   NumSamples <- ceiling(2*((Z1MinusA + Z1MinusB)*StdDev/Delta)<sup>2</sup> +
       0.25*Z1MinusA^2)
   # Put numbers in correct format
   cat(paste(
                PadL(i,2),
                 PadR(Alpha,4,"0"),
                 PadR(Beta, 4, "0"),
                 PadR(Delta,4,"0"),
                 PadR(StdDev, 4, "0"),
                 PadL(NumSamples,4),"XXXX",sep=",\t\t"),"\n")
}
#----- Tests of Confidence Interval for a Mean -----
cat("\nTests of Confidence Interval for a Mean\n")
             Type Conf. Level StdDev. 1/2 Width Test n VSP n\n")
cat("Case
# Force the same string of "random" numbers each time
set.seed(4)
# Generate NumCases random test cases
for(i in 1:NumCases) {
   ConfLevl <- round(runif(1, .50, .99), digits=2)</pre>
   Type
             <- ifelse(runif(1) > 0.5, "Two-Sided", "One-Sided")
             <- round(runif(1, 0.5, 10.0), digits=2)
   StdDev
   Delta <- round(runif(1, 0.1, 2.0), digits=2)</pre>
   if (Type == "Two-Sided") {
      UseConfLevl <- 0.5 + ConfLevl/2
   } else {
       # One-Sided Case
       UseConfLevl <- ConfLevl
   # Calculate sample size using Gilbert 1997, p. 32
   dNumZ <- ceiling((qnorm(UseConfLevl)*StdDev/Delta)^2)</pre>
   if (dNumZ <= 2.0) {dNumZ <- 2.0}
   dNum1 <- dNumZ
   nTrial <- 0
   while (T) {
       nTrial <- nTrial + 1
       dt <- qt(UseConfLev1, dNum1-1)</pre>
       dNum2 <- dt * StdDev/Delta
       dNum2 <- ceiling(dNum2 * dNum2)</pre>
       dNum1 <- ceiling((dNum2 + dNum1)/2)</pre>
       if (abs(dNum2-dNum1) <= 1.0) {
          break
       }
   }
   NumSamples
                 <- dNum1
   # Put numbers in correct format
   cat(paste(
                 PadL(i,2),
                 Type,
                 PadR(ConfLevl,4,"0"),
                 PadR(StdDev,4,"0"),
                 PadR(Delta,4,"0"),
                 PadL(NumSamples,4),"XXXX",sep=",\t\t"),"\n")
}
```

```
#---- Tests of Mean (or Median) vs. Action Level: Wilcoxon Signed Rank Test Equation
cat("\nTests of Mean (or Median) vs. Action Level:",
   "Wilcoxon Signed Rank Test Equation\n")
           Alpha Beta Delta StdDev. Test n VSP n\n")
cat("Case
# Force the same string of "random" numbers each time
set.seed(4)
# Generate NumCases random test cases
for(i in 1:NumCases) {
   Alpha
             <- round(runif(1, .01, .25), digits=2)
   Beta
             <- round(runif(1, .01, .25), digits=2)
   Delta <- round(runif(1, .1, 5.0), digits=2)</pre>
            <- round(runif(1, 0.5, 10.0), digits=2)
   StdDev
   Z1MinusA <- qnorm(1.0 - Alpha)
   Z1MinusB <- qnorm(1.0 - Beta)
   # Calculate sample size using EPA 1996, p. 3.2-8
   NumSamples <- ceiling(1.16*(((Z1MinusA + Z1MinusB)*StdDev/Delta)<sup>2</sup> +
      0.5*Z1MinusA^2))
   # Put numbers in correct format
                PadL(i,2),
   cat(paste(
                PadR(Alpha,4,"0"),
                PadR(Beta, 4, "0"),
                PadR(Delta,4,"0")
                PadR(StdDev,4,"0"),
                PadL(NumSamples,4), "XXXX", sep=", \t\t"), "\n")
}
#---- Tests of Proportion vs. Given Proportion: One-Sample Proportion Test ----
cat("\nTests of Proportion vs. Given Proportion: One-Sample Proportion Test\n")
cat("Case
            Alpha
                     Beta Delta PO
                                                 Test n VSP n n'
# Force the same string of "random" numbers each time
set.seed(4)
# Generate NumCases random test cases
for(i in 1:NumCases) {
             <- round(runif(1, .01, .25), digits=2)
   Alpha
             <- round(runif(1, .01, .25), digits=2)
   Beta
   Delta <- round(runif(1, .01, .49), digits=2)</pre>
             <- round(runif(1, .01, .99), digits=2)
   P0
   Ρ1
             <- P0 - Delta
   # Below is meant to duplicate the way VSP deals with Delta
   if (P1 < 0.0) {
      P1 <- 0.001
      Delta <- P0 - P1
   }
   Z1MinusA <- qnorm(1.0 - Alpha)
   Z1MinusB <- qnorm(1.0 - Beta)
   # Calculate sample size using EPA 1996, p. 3.2-12
               <- ceiling(((Z1MinusA*sqrt(P0*(1.0-P0)) +
   NumSamples
      Z1MinusB*sqrt(P1*(1.0-P1)))/Delta)<sup>2</sup>
   # Put numbers in correct format
   cat(paste(
                PadL(i,2),
                PadR(Alpha,4,"0"),
                PadR(Beta, 4, "0"),
                PadR(Delta,5,"0"),
                PadR(P0,4,"0"),
                PadL(NumSamples,4),"XXXX",sep=",\t\t"),"\n")
}
#---- Tests of Two Proportions: Two-Sample Test for Proportions -----
cat("\nTests of Two Proportions: Two-Sample Test for Proportions\n")
cat("Case
           Alpha
                    Beta Delta
                                      P1
                                                  P2
                                                           Test n VSP n\n")
# Force the same string of "random" numbers each time
set.seed(4)
```

```
# Generate NumCases random test cases
for(i in 1:NumCases) {
             <- round(runif(1, .01, .25), digits=2)
   Alpha
   Beta
              <- round(runif(1, .01, .25), digits=2)
   Delta <- round(runif(1, .01, .50), digits=2)</pre>
             <- round(runif(1, .00, .99), digits=2)
   P2
   # Choose P1 so that PAver is closest to 0.5. Also, P1 must be positive
   if (P2 <= 0.5) {
      P1 <- P2 + Delta
   } else {
      P1 <- P2 - Delta
   PAver
             <- 0.5 * (P1 + P2)
   Z1MinusA <- qnorm(1.0 - Alpha)
   Z1MinusB <- qnorm(1.0 - Beta)
   # Calculate sample size using EPA 1996, p. 3.3-8
   NumSamples <- ceiling((2*(Z1MinusA + Z1MinusB)<sup>2</sup>*PAver*(1.0-PAver))/Delta<sup>2</sup>)
   # Put numbers in correct format
   cat(paste( PadL(i,2),
                 PadR(Alpha,4,"0"),
                 PadR(Beta, 4, "0"),
                 PadR(Delta,4,"0"),
                 PadR(P1,4,"0"),
                 PadR(P2,4,"0"),
                 PadL(NumSamples,4), "XXXX", sep=", \t\t"), "\n")
}
#----- Tests of Two Populations: QA/G-9 Wilcoxon Rank Sum Test -----
cat("\nTests of Two Populations: QA/G-9 Wilcoxon Rank Sum Test\n")
cat("Case
            Alpha
                     Beta Delta
                                       StdDev. Test n VSP n n")
# Force the same string of "random" numbers each time
set.seed(4)
# Generate NumCases random test cases
for(i in 1:NumCases) {
             <- round(runif(1, .01, .25), digits=2)
   Alpha
   Beta<- round(runif(1, .01, .25), digits=2)</td>Delta<- round(runif(1, .1, 5.0), digits=2)</td>StdDev<- round(runif(1, 0.5, 10.0), digits=2)</td>
   Z1MinusA <- qnorm(1.0 - Alpha)
   Z1MinusB <- qnorm(1.0 - Beta)
   # Calculate sample size using EPA 1996, pp. 3.3-10 to 3.3-12
   NumSamples <- ceiling(1.16*(2*StdDev^2*(Z1MinusA + Z1MinusB)^2/Delta^2 +
       0.25*Z1MinusA^2))
   # Put numbers in correct format
                 PadL(i,2),
   cat(paste(
                 PadR(Alpha,4,"0"),
                 PadR(Beta, 4, "0"),
                 PadR(Delta,4,"0"),
                 PadR(StdDev,4,"0"),
                 PadL(NumSamples,4),"XXXX",sep=",\t\t"),"\n")
}
#---- Tests of MARSSIM Sign Test: Comparison of Median vs. Action Level -----
cat("\nTests of MARSSIM Sign Test: Comparison of Median vs. Action Level\n")
                     Beta Delta StdDev. SignP
cat("Case
            Alpha
                                                               Test n VSP n\n")
# Force the same string of "random" numbers each time
set.seed(4)
# Generate NumCases random test cases
for(i in 1:NumCases) {
             <- round(runif(1, .01, .25), digits=2)
   Alpha
   Beta
              <- round(runif(1, .01, .25), digits=2)
   Delta <- round(runif(1, .1, 5.0), digits=2)</pre>
   StdDev <- round(runif(1, 0.5, 10.0), digits=2)</pre>
```

```
<- pnorm(Delta/StdDev)
   SiqnP
   Z1MinusA <- qnorm(1.0 - Alpha)</pre>
   Z1MinusB <- qnorm(1.0 - Beta)
   # Calculate sample size using MARSSIM p. 5-33
   NumSamples <- ceiling((Z1MinusA + Z1MinusB)<sup>2</sup>/(4*(SignP - 0.5)<sup>2</sup>))
   # Put numbers in correct format
   SignP <- round(SignP, digits=3)</pre>
                 PadL(i,2),
   cat(paste(
                  PadR(Alpha,4,"0"),
                  PadR(Beta, 4, "0"),
                  PadR(Delta,4,"0"),
                  PadR(StdDev,4,"0"),
                  PadR(SignP,5,"0"),
                  PadL(NumSamples,4),"XXXX",sep=",\t\t"),"\n")
}
#---- Tests of MARSSIM WRS Test: Comparison of Median vs. Background Level ----
cat("\nTests of MARSSIM WRS Test: Comparison of Median vs. Background Level\n")
cat("Case Alpha
                     Beta Delta StdDev. Pr
                                                                Test n
                                                                         VSP n∖n")
# Force the same string of "random" numbers each time
set.seed(4)
# Generate NumCases random test cases
for(i in 1:NumCases) {
              <- round(runif(1, .01, .25), digits=2)
   Alpha
   Beta <- round(runif(1, .01, .25), digits=2)
Delta <- round(runif(1, .1, 5.0), digits=2)</pre>
              <- round(runif(1, 0.5, 10.0), digits=2)
   StdDev
   Pr
              <- pnorm(Delta/(sqrt(2)*StdDev))
   Z1MinusA <- qnorm(1.0 - Alpha)
   Z1MinusB <- qnorm(1.0 - Beta)</pre>
   # Calculate sample size using MARSSIM p. 5-28
   NumSamples <- ceiling((Z1MinusA + Z1MinusB)<sup>2</sup>/(3.0*(Pr - 0.5)<sup>2</sup>)/2)
   # Put numbers in correct format
   Pr <- round(Pr, digits=3)</pre>
                 PadL(i,2),
   cat(paste(
                  PadR(Alpha,4,"0"),
                  PadR(Beta, 4, "0"),
                  PadR(Delta,4,"0"),
                  PadR(StdDev,4,"0"),
                  PadR(Pr, 5, "0"),
                  PadL(NumSamples,4),"XXXX",sep=",\t\t"),"\n")
}
cat("End run: VSPTest\n")
sink()
cat("End run: VSPTest\n")
}
```

```
"PadL" <- function(Item, nWidth=4, cPad=" ")
{
# Function: PadL
# Purpose.: Pads a string or numeric item with cPad on the left
# Usage...: Item <- PadL(Item, 5) makes Item 5 wide using spaces on left
# Started.: 06/09/99
# Last Mod: 06/09/99
# Author..: Jim Davidson, Battelle PNNL Statistics Group
nLen <- nchar(Item)</pre>
if (nLen < nWidth) {
  cPad <- paste(rep(cPad,nWidth-nLen),sep="", collapse="")
  Item <- paste(cPad,Item,sep="")</pre>
}
return(Item)
}
"PadR" <- function(Item, nWidth=4, cPad=" ")
#______
# Function: PadR
# Purpose.: Pads a string or numeric item with cPad on the right
# Usage...: Item <- PadR(Item, 5) makes Item 5 wide using spaces on right
# Started.: 06/09/99
# Last Mod: 06/09/99
# Author..: Jim Davidson, Battelle PNNL Statistics Group
nLen <- nchar(Item)</pre>
if (nLen < nWidth) {
  cPad <- paste(rep(cPad,nWidth-nLen),sep="", collapse="")
  Item <- paste(Item, cPad, sep="")</pre>
}
return(Item)
}
```

Appendix C Input File of Singer's 100 Test Cases

# Appendix C Input File of Singer's 100 Test Cases

Test100.SIF, an SIF format input test file for HOTSPOT, 02/06/94. \* This sample SIF (Simplified Input Format) file illustrates the format specs: \* (1) The 1st line in the file is always the title line, \* just as in an ELIPGRID formated input file. \* (2) Any line can be commented by using an asterisk, \*, as the 1st nonblank character. \* (3) The data values must be separated by 1 or more spaces. (4) They must come in the order shown below, but the 2nd, 3rd, & 4th data rows below illustrate that between-column spacing does not matter. \* (5) No worries with column spacing is what makes this format "simple" in contrast to ELIPGRID's rigid FORTRAN style column format. \* \* (6) Note that for rectangular grids, the long/short side ratio follows the data line as in ELIPGRID. However, it need not be in columns 1-10. \* (7) End of File can now be either Shape > 1, as in ELIPGRID's format, or simply no more data lines in the file. \* Semimajor Shape Angle GridSize Type Orient. TargetID 1000.0 0.38 22.0 800.0 1 0 #261 \* Note how next 3 lines do not match ELIPGRID's column format. 0.30 6.0 800.0 1 0 #187 1250.0 38.0 1250.0 0.50 800.0 1 0 #190 300.0 0.25 24.0 800.0 1 0 #147 625.0 0.50 35.0 800.0 1 0 #10 875.0 0.31 800.0 #19 7.0 1 0 625.0 0.20 18.0 800.0 1 0 #26 125.0 0.50 24.0 800.0 1 0 #30 1625.0 0.15 11.0 800.0 1 0 #49 1250.0 0.50 0.0 800.0 1 0 #104 22.0 1000.0 0.38 1000.0 1 0 #261 1250.0 0.30 6.0 1000.0 1 0 #187 1000.0 1 1250.0 0.50 38.0 0 #190 300.0 0.25 24.0 1000.0 1 0 #147 625.0 0.50 35.0 1000.0 1 0 #10 1000.0 1 875.0 7.0 0 0.31 #19 625.0 0.20 18.0 1000.0 1 0 #26 125.0 0.50 24.0 1000.0 1 0 #30 1 1625.0 0.15 11.0 1000.0 0 #49 1 1000.0 1250.0 0.50 0.0 0 #104 1000.0 0.38 22.0 1500.0 0 #261 1 1250.0 0.30 6.0 1500.0 1 0 #187 0.50 38.0 1500.0 1250.0 1 0 #190 0.25 24.0 1500.0 300.0 1 0 #147 625.0 0.50 35.0 1500.0 0 #10 1 875.0 0.31 7.0 1500.0 1 0 #19 625.0 0.20 18.0 1500.0 1 0 #26 125.0 0.50 24.0 1500.0 0 #30 1 1625.0 0.15 11.0 1500.0 1 0 #49 1250.0 0.50 0.0 1500.0 1 0 #104 1000.0 0.38 22.0 859.66 2 0 #261 0.30 6.0 859.66 2 0 #187 1250.0 0.50 22.0 859.66 2 0 #190 1250.0 625.0 0.50 35.0 565.69 3 0 #10 2.0 875.0 0.31 7.0 565.69 3 0 #19 2.0 625.0 0.20 18.0 565.69 3 0 #26 2.0 125.0 0.50 24.0 0 #30 565.69 3

2.0 1625.0	0.15	11.0	565.69	3	0	#49
2.0 1250.0	0.50	0.0	565.69	3	0	#104
2.0 1000.0	0.38	22.0	707.11	3	0	#261
2.0 1250.0	0.30	6.0	707.11	3	0	#187
2.0						
1250.0 2.0	0.50	38.0	707.11	3	0	#190
300.0 2.0	0.25	66.0	707.11	3	0	#147
625.0 2.0	0.50	35.0	707.11	3	0	#10
875.0 2.0	0.31	7.0	707.11	3	0	#19
625.0	0.20	18.0	707.11	3	0	#26
2.0 125.0	0.50	24.0	707.11	3	0	#30
2.0 1625.0	0.15	11.0	707.11	3	0	#49
2.0 1250.0	0.50	0.0	707.11	3	0	#104
2.0 1000.0	0.38	22.0	1060.66	3	0	#261
2.0 1250.0	0.30	6.0	1060.66	3	0	#187
2.0						
300.0	0.25	6.0	859.66	2	0	#147
625.0	0.50	25.0	859.66	2	0	#10
875.0	0.31	7.0	859.66	2	0	#19
625.0	0.20	18.0	859.66	2	0	#26
125.0	0.50	24.0	859.66	2	0	#30
1625.0	0.15	11.0	859.66	2	0	#49
1250.0	0.50	0.0	859.66	2	0	#104
1000.0	0.38	22.0	1074.57	2	0	#261
1250.0	0.30	6.0	1074.57	2	0	#187
1250.0	0.50	22.0	1074.57	2	0	#190
300.0	0.25	6.0	1074.57	2	0	#147
625.0	0.50	25.0	1074.57	2	0	#10
875.0	0.31	7.0	1074.57	2	0	#19
625.0	0.2	18.0	1074.57	2	0	#26
125.0	0.50	24.0	1074.57	2	0	
						#30
1625.0	0.15	11.0	1074.57	2	0	#49
1250.0	0.50	0.0	1074.57	2	0	#104
1000.0	0.38	22.0	1611.86	2	0	#261
1250.0	0.30	6.0	1611.86	2	0	#187
1250.0	0.50	22.0	1611.86	2	0	#190
300.0	0.25	6.0	1611.86	2	0	#147
625.0	0.50	25.0	1611.86	2	0	#10
875.0	0.31	7.0	1611.86	2	0	#19
625.0	0.20	18.0	1611.86	2	0	#26
125.0	0.50	24.0	1611.86	2	0	#30
						#49
1625.0	0.15	11.0	1611.86	2	0	
1250.0	0.50	0.0	1611.86	2	0	#104
1000.0	0.38	22.0	565.69	3	0	#261
2.0						
1250.0	0.30	6.0	565.69	3	0	#187
2.0						
1250.0	0.50	38.0	565.69	3	0	#190
2.0						
300.0	0.25	66.0	565.69	3	0	#147

2.0						
1250.0	0.50	38.0	1060.66	3	0	#190
2.0						
300.0	0.25	66.0	1060.66	3	0	#147
2.0						
625.0	0.50	35.0	1060.66	3	0	#10
2.0				_	_	
875.0	0.31	7.0	1060.66	3	0	#19
2.0	0.00	10 0	1000 00	2	0	# <b>D</b> C
625.0 2.0	0.20	18.0	1060.66	3	0	#26
125.0	0.50	24.0	1060.66	3	0	#30
2.0	0.50	24.0	1000.00	J	0	#50
1625.0	0.15	11.0	1060.66	3	0	#49
2.0						
1250.0	0.50	0.0	1060.66	3	0	#104
2.0						
1000.0	0.38	22.0	1000.0	1	1	#261
1250.0	0.30	6.0	1000.0	1	1	#187
1250.0	0.50	38.0	1000.0	1	1	#190
300.0	0.25	24.0	1000.0	1	1	#147
625.0	0.50	35.0	1000.0	1	1	#10
875.0	0.31	7.0	1000.0	1	1	#19
625.0	0.20	18.0	1000.0	1	1	#26
125.0	0.50	24.0	1000.0	1	1	#30
1625.0	0.15	11.0	1000.0	1	1	#49
1250.0	0.50	0.0	1000.0	1	1	#104
9.9	9.9	9.9	9.9	9	9	EOF

Appendix D VSP Output File for Singer's 100 Test Cases

# Appendix D VSP Output File for Singer's 100 Test Cases

Output from Visual Sample Plan Fortran Test Code Version: 04/29/99 File Name.: Test100.Out Created on: 06/17/1999 Input file: Test100.Sif using SIF format. Title line: Test100.SIF, an SIF format input test file for HOTSPOT, 02/06/94.

Target	Grid Type		-major Axis lative Units	Gridspace in Orig Units	Shape	Angle	Prob(0)
#261	Square	III KC	1.2500	800.00	0.38	22.0	0.0000
#187	Square		1.5625	800.00	0.30	6.0	0.0311
#190	Square		1.5625	800.00	0.50	38.0	0.0000
#190 #147	Square		0.3750	800.00	0.25	24.0	0.8896
#10	Square		0.7813	800.00	0.50	35.0	0.0906
#10 #19	Square		1.0938	800.00	0.31	7.0	0.3059
#26	Square		0.7813	800.00	0.20	18.0	0.6165
#20	Square		0.1563	800.00	0.50	24.0	0.9617
#30 #49	Square		2.0313	800.00	0.15	11.0	0.0470
#104	Square		1.5625	800.00	0.50	0.0	0.0000
#261	Square		1.0000	1000.00	0.38	22.0	0.0619
#187	Square		1.2500	1000.00	0.30	6.0	0.2337
#190 #190	Square		1.2500	1000.00	0.50	38.0	0.0000
#190 #147	Square		0.3000	1000.00	0.25	24.0	0.9293
#10	Square		0.6250	1000.00	0.50	35.0	0.3864
#10 #19	Square		0.8750	1000.00	0.31	7.0	0.4591
#26	Square		0.6250	1000.00	0.20	18.0	0.7546
#20	Square		0.1250	1000.00	0.50	24.0	0.9755
#30 #49	Square		1.6250	1000.00	0.15	11.0	0.2499
#104	Square		1.2500	1000.00	0.50	0.0	0.0000
#104 #261	Square		0.6667	1500.00	0.38	22.0	0.4694
#187	Square		0.8333	1500.00	0.30	6.0	0.5107
#190 #190	Square		0.8333	1500.00	0.50	38.0	0.0266
#190 #147	Square		0.2000	1500.00	0.25	24.0	0.9686
#10	Square		0.4167	1500.00	0.50	35.0	0.7273
#10 #19	Square		0.5833	1500.00	0.31	7.0	0.6783
#26	Square		0.4167	1500.00	0.20	18.0	0.8909
#20	Square		0.0833	1500.00	0.50	24.0	0.9891
#49	Square		1.0833	1500.00	0.15	11.0	0.5307
#104	Square		0.8333	1500.00	0.50	0.0	0.2198
#261	Triangular		1.1633	859.66	0.38	22.0	0.0000
#187	Triangular		1.4541	859.66	0.30	6.0	0.0000
#190	Triangular		1.4541	859.66	0.50	22.0	0.0000
#10	Rectangular,	2.0/1	1.1048	565.69	0.50	35.0	0.1518
#19	Rectangular,	2.0/1	1.5468	565.69	0.31	7.0	0.0646
#26	Rectangular,	2.0/1	1.1048	565.69	0.20	18.0	0.6165
#30	Rectangular,	2.0/1	0.2210	565.69	0.50	24.0	0.9617
#49	Rectangular,	2.0/1	2.8726	565.69	0.15	11.0	0.0000
#104	Rectangular,	2.0/1	2.2097	565.69	0.50	0.0	0.0000
#261	Rectangular,	2.0/1	1.4142	707.11	0.38	22.0	0.0022
#187	Rectangular,	2.0/1	1.7678	707.11	0.30	6.0	0.0000
#190	Rectangular,	•	1.7678	707.11	0.50		0.0000
#147	Rectangular,	2.0/1	0.4243	707.11	0.25	66.0	0.9293
#10	Rectangular,	2.0/1	0.8839	707.11	0.50	35.0	0.3882
#19	Rectangular,	2.0/1	1.2374	707.11	0.31	7.0	0.2989
#26	Rectangular,	2.0/1	0.8839	707.11	0.20	18.0	0.7546
#30	Rectangular,	2.0/1	0.1768	707.11	0.50	24.0	0.9755
#49	Rectangular,	2.0/1	2.2981	707.11	0.15	11.0	0.0090
#104	Rectangular,	2.0/1	1.7678	707.11	0.50	0.0	0.0000
#261	Rectangular,	2.0/1	0.9428	1060.66	0.38	22.0	0.4694
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		/ -					
#187	Rectangular,	2.0/1	1.1785	1060.66	0.30	6.0	0.3721
#147	Triangular		0.3490	859.66	0.25	6.0	0.8896
#10	Triangular		0.7270	859.66	0.50	25.0	0.1113
#19	Triangular		1.0178	859.66	0.31	7.0	0.2594
#26	Triangular		0.7270	859.66	0.20	18.0	0.6165
#30	Triangular		0.1454	859.66	0.50	24.0	0.9617
#49	Triangular		1.8903	859.66	0.15	11.0	0.0023
#104	Triangular		1.4541	859.66	0.50	0.0	0.0000
#261	Triangular		0.9306	1074.57	0.38	22.0	0.0134
#187	Triangular		1.1633	1074.57	0.30	6.0	0.1807
#190	Triangular		1.1633	1074.57	0.50	22.0	0.0000
#147	Triangular		0.2792	1074.57	0.25	6.0	0.9293
#10	Triangular		0.5816	1074.57	0.50	25.0	0.3864
#10 #19	Triangular		0.8143	1074.57	0.31	7.0	0.4257
	-						
#26	Triangular		0.5816	1074.57	0.20	18.0	0.7546
#30	Triangular		0.1163	1074.57	0.50	24.0	0.9755
#49	Triangular		1.5122	1074.57	0.15	11.0	0.1998
#104	Triangular		1.1633	1074.57	0.50	0.0	0.0000
#261	Triangular		0.6204	1611.86	0.38	22.0	0.4694
#187	Triangular		0.7755	1611.86	0.30	6.0	0.4810
#190	Triangular		0.7755	1611.86	0.50	22.0	0.0677
#147	Triangular		0.1861	1611.86	0.25	6.0	0.9686
#10	Triangular		0.3878	1611.86	0.50	25.0	0.7273
#19	Triangular		0.5429	1611.86	0.31	7.0	0.6695
#26	Triangular		0.3878	1611.86	0.20	18.0	0.8909
#30	Triangular		0.0776	1611.86	0.50	24.0	0.9891
#49	Triangular		1.0082	1611.86	0.15	11.0	0.5058
#104	Triangular		0.7755	1611.86	0.50	0.0	0.1712
#261	Rectangular,	2.0/1	1.7678	565.69	0.38	22.0	0.0000
#187	Rectangular,	2.0/1	2.2097	565.69	0.30	6.0	0.0000
#190	Rectangular,	2.0/1	2.2097	565.69	0.50	38.0	0.0000
#147	Rectangular,	2.0/1	0.5303	565.69	0.25	66.0	0.8896
#190	Rectangular,	2.0/1	1.1785	1060.66	0.50	38.0	0.0969
#190 #147	Rectangular,	2.0/1	0.2828	1060.66	0.25	66.0	0.9686
	-						
#10 #10	Rectangular,	2.0/1	0.5893	1060.66	0.50	35.0	0.7273
#19	Rectangular,	2.0/1	0.8250	1060.66	0.31	7.0	0.6686
#26	Rectangular,	2.0/1	0.5893	1060.66	0.20	18.0	0.8909
#30	Rectangular,	2.0/1	0.1179	1060.66	0.50	24.0	0.9891
#49	Rectangular,	2.0/1	1.5321	1060.66	0.15	11.0	0.4469
#104	Rectangular,	2.0/1	1.1785	1060.66	0.50	0.0	0.0600
#261	Square		1.0000	1000.00	0.38	Random	0.1137
#187	Square		1.2500	1000.00	0.30	Random	0.0730
#190	Square		1.2500	1000.00	0.50	Random	0.0000
#147	Square		0.3000	1000.00	0.25	Random	0.9293
#10	Square		0.6250	1000.00	0.50	Random	0.4072
#19	Square		0.8750	1000.00	0.31	Random	0.3474
#26	Square		0.6250	1000.00	0.20	Random	0.7577
#30	Square		0.1250	1000.00	0.50	Random	0.9755
#49	Square		1.6250	1000.00	0.15	Random	0.1835
#104	Square		1.2500	1000.00	0.50	Random	0.0000
	<b>⊥</b> .						

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