Summary Analysis of a Monte Carlo Simulation of Ecology's Statistical Guidance and a Proposed Alternative

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1.0 INTRODUCTION

The State of Washington has recommended a specific statistical test procedure for identifying soil contamination at a potential waste site (Ecology 1992), referred to here as the State test. An alternative to this test has been presented (DOE/RL 1994), which uses the Wilcoxon Rank Sum, Quantile, and Hot Measurement Comparison tests (WQH). These same tests are recommended by the U.S. Environmental Protection Agency (EPA) to determine if soils from a waste site differ from site-specific, reference-based standards (EPA 1994).

In support of employing the WQH test as an alternative to the State test, as allowed in *Washington Administrative Code* 173-340-740 (7) (d) (iii), Monte Carlo simulations comparing the performance of the State test with the Wilcoxon Rank Sum and Quantile tests have been conducted for a range of conditions. A large number of these simulations have been conducted and reported by Hardin and Gilbert (1993). Reviews of the WQH test procedure by the Washington State Department of Ecology (Ecology) and discussions with Ecology, EPA, and the Washington State Department of Health have led to a request for additional Monte Carlo simulations. This request was directed at meeting the following requirements:

- Combine the Wilcoxon, Quantile, and Hot Measurement tests and measure their performance against the State test.
- Provide power curves in which the WQH procedure and the State test have equivalent Type I error rates.
- Provide additional resolution in the variable space of the simulation, particularly with respect to small sample sizes and coefficients of variation (CV).

2.0 TEST PROCEDURE

The original analysis performed by Hardin and Gilbert (1993) was based on a fixed Type I error rate of 5%, as specified in Ecology's statistical guidance (Ecology 1992). Unfortunately, Ecology's procedure did not reproduce the specified Type I error rate, and occasionally yielded excessively large error rates (>20%). The actual Type I error rates were reported along with the full power curves for the simulation. The recommendations in Hardin and Gilbert (1993) were based on the ability to reproduce the specified Type I error rate and the power of the test.

Discussions with Ecology led to the need to directly compare Ecology's procedure with the recommended alternative at the same Type I error rates actually achieved by the procedures. This led to the following simulation procedure:

1. The YORIC code (Hardin and Gilbert 1993) was run to estimate the total Type I error rates for both the State test and the WQH combination, based on $N = 1,000$ trials for each

combination of simulation parameters. The total error rates were compared and the specified Type I error rates for the Wilcoxon and Quantile tests were scaled (equally), so that the total Type I error rates between the State test and the WQH combination were equivalent.

2. The Type I error rates for the State test and the WQH were again estimated by the method described in Step 1. If the error rates were found equivalent, then the full simulation process, described below, was implemented. If the Type I error rates were not equivalent, they were adjusted and run again, as in Step 1.

The iterative process for matching the Type I error rates used the following equation for adjusting the specified Wilcoxon and Quantile Type I error rates:

$$\alpha_{n+1} = \frac{\alpha_{\text{State test}}}{\alpha_{\text{WQH}}} \alpha_n \quad (1)$$

where α_n is the current specification and α_{n+1} is the updated specification. The initial α level for the Wilcoxon and Quantile tests was set to 0.05, and the iteration process was terminated when the individual Type I error rates agreed within 1 standard deviation of the estimate of the total State test Type I error rate. This can be expressed by the following equation:

$$|\alpha_n - \alpha_{n+1}| \leq \delta = \sqrt{\frac{\alpha_{\text{state}}(1 - \alpha_{\text{state}})}{N_{\text{trials}}}} \quad (2)$$

Once the Type I error rates were matched, the YORIC code was then run for the full suite of parameters with the State test having a specified Type I error rate of 5%, and the Wilcoxon and Quantile tests having individually specified Type I error rates determined from the above procedure. This provided a common basis for comparing the resulting power curves.

The following parameters were used for the simulations:

N = Number of trials	=	10,000
m = number of background samples	=	10, 20, 30, 50
n = Number of waste site samples	=	10, 20, 30, 50
ϵ = fraction of waste site contaminated	=	0.1, 0.5, 1.0
CV = Coefficient of Variation (Standard Deviation/Mean)	=	0.1, 0.3, 0.5, 0.7, 1.0
P_r = Probability of Exceedance	=	0.50, 0.55, 0.60, 0.65
$P_{(\text{background datum} < \text{waste site datum})}$	=	0.70, 0.75, 0.80, 0.85
	=	0.90, 0.95, 0.99, 0.999
TYPE = Distribution type	=	Lognormal, Weibull

The fraction of waste site contaminated, ϵ , is the fraction of the total number of site samples that are collected from the contaminated portion of the site. Consequently, $1-\epsilon$ is the fraction collected from the portion of the site that is not contaminated greater than the background area.

The probability of exceedance, P_e , is the probability that a random value drawn from the contaminated distribution is greater than a random value drawn from the background distribution. The $P_e = 0.5$ when $\epsilon = 0$ (i.e., when the site and background distributions are identical). The P_e approaches 1 as ϵ becomes greater than 0 (i.e., as the contaminated distribution is shifted more to the right from the background distribution). More detailed descriptions of the parameters and how they were used in the YORIC simulations can be found in Hardin and Gilbert (1993), along with a discussion of the hypothesis test and error structure used in these tests.

All combinations of parameters were used in the simulations, producing 480 separate power curves. These parameters were selected to focus on small sample sizes and the coefficient of variation as key parameters for the analysis. The power curves are contained in this report as Attachment A (for the Lognormal distribution) and Attachment B (for the Weibull distribution).

3.0 RESULTS

The WQH alternative generally displays a power equal or superior to the State test, with some limited exceptions. For $\epsilon = 0.1$, neither test has a high power and they are generally equivalent. The State test has higher power over a narrow range of conditions, namely in a lognormal distribution when background sample size is small ($n=10$), $\epsilon = 0.5$, and CV is low (0.1 to 0.3). These conditions formed the original design basis of the State test.

The advantage of the State test, under the above conditions, disappears as background sample size increases above 20 and when CV and/or ϵ are increased. As ϵ approaches 1.0, the WQH has a higher power under almost all conditions. The increased power of the State test, relative to the WQH under the above conditions, is also diminished when the populations are drawn from a Weibull distribution.

4.0 DISCUSSION

Evaluation of the use of the State test over the WQH alternative is influenced by the following factors:

1. The number of background samples collected by the Sitewide Background Project is seldom less than fifty and quite often much greater. This immediately eliminates the power advantage of the State test noted above and establishes the WQH as a preferred alternative.

2. Ecology has recommended, in comment resolution discussions for DOE/RL-94-72, that stratification (of the waste site area to be sampled) be used "to reduce statistical dilution of contamination." This amounts to using expert judgment and *a priori* information to drive ϵ to 1.0, for which the WQH combination is the superior method.
3. A critical performance area for the analysis procedure is in validation of a remediation effort. If a preferred action is removal of contamination, the remediation effort will drive ϵ towards 0 and away from the value of 0.5, the condition at which the State test's performance surpasses that of the WQH. At $\epsilon = 0.1$, there is no advantage to either test.
4. The State test Type I error rate is erratic and essentially uncontrolled. Even though the analyst specifies a Type I error rate of 0.05 (as recommended by Ecology) the actual Type I error rate will be something larger and generally unknown. "Correcting" for this problem by specifying a smaller Type I error rate is not possible because it requires the following:
 - A unique specification of a reduced α for each application, since the reduction is dependent on m , n , CV, and distribution type.
 - Information not currently in the Ecology statistical guidance (e.g., Supplement S-2 in Ecology, 1992) to derive values for $H_{1-\alpha}$ at the analysis-specific reduced α level.
5. The EPA (1994) has adopted the WQH combination of tests as an appropriate procedure for determining the attainment of background-based cleanup standards.
6. The NRC (1995) recommends that the WQH combination be used for NRC license termination when radionuclides of concern are present in the background.
7. The U.S. Department of Defense, EPA, NRC, and DOE are jointly developing a Multi-Agency Site Investigation and Remediation Manual (MARSIM, currently in internal review) to provide consistent guidance across the principal federal agencies dealing with federal facility cleanup efforts. The NRC statistical guidance (NRC 1995) is proposed to be included in the MARSIM.

Based on these factors, DOE is recommending that the combination procedure of the Wilcoxon, Quantile, and Hot Measurement tests be used instead of the State test for determining the presence of contamination compared to background. The WQH combination test is consistently more powerful when the number of background samples available is 50 or more, which is the case when the Hanford Site background data set is used.

5.0 REFERENCES

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- Ecology, 1992, *Statistical Guidance for Ecology Site Managers*, DOE/RL-92-54, Washington State Department of Ecology, Lacey, Washington.
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- Hardin, J. W. and R. O. Gilbert, 1993, *Comparing Statistical Tests for Detecting Soil Contamination Greater Than Background*, PNL-8989, Pacific Northwest Laboratory, Richland, Washington.
- NRC, 1995, *A Non-Parametric Statistical Methodology for the Design and Analysis of Final Status Decommissioning Surveys*, NUREG-1505, Draft Report for Comment, U.S. Nuclear Regulatory Commission, Washington, D.C.

ATTACHMENT A

Power Curve Plots of Monte Carlo Simulations for the State and the WQH tests, Using a Lognormal Distribution.

EXPLANATION

The plots contained in this attachment compare the performance of the State and WQH tests for a range of conditions, as described in the text. In all of the plots, the x-axis (abscissa) is the probability of exceedance (P_e), and the y-axis (ordinate) is the probability that the test indicates that the site is contaminated.

- 10 = Number of background samples
- 10 = Number of site samples
- 10000 = Number of iterations in simulation
- 0.1 = Coefficient of variation of background distribution
- 100 = Mean of background distribution
- 0.05 = Desired level of significance (line included in plots)
- e = Amount of mixture between distributions
- Lognormal = Background (and shifted) distribution

The background sample is derived from the indicated distribution with the given mean and coefficient of variation. A second distribution is then defined as a pure shift from the background distribution. It is defined in terms of P_r which measures the probability that a random

value from the background is less than a random value from the shifted distribution. The site samples are drawn from a mixture of the background and shifted distributions. The proportion of the shifted distribution in the derivation of the site sample mixture distribution is given by the value of epsilon (e).

- 20 = Number of background samples
- 10 = Number of site samples
- 10000 = Number of iterations in simulation
- 0.1 = Coefficient of variation of background distribution
- 100 = Mean of background distribution
- 0.05 = Desired level of significance (line included in plots)
- e = Amount of mixture between distributions
- Lognormal = Background (and shifted) distribution

The background sample is derived from the indicated distribution with the given mean and coefficient of variation. A second distribution is then defined as a pure shift from the background distribution. It is defined in terms of Pr which measures the probability that a random

value from the background is less than a random value from the shifted distribution. The site samples are drawn from a mixture of the background and shifted distributions. The proportion of the shifted distribution in the derivation of the site sample mixture distribution is given by the value of e .

- 30 = Number of background samples
- 10 = Number of site samples
- 10000 = Number of iterations in simulation
- 0.1 = Coefficient of variation of background distribution
- 100 = Mean of background distribution
- 0.05 = Desired level of significance (line included in plots)
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- 50 = Number of background samples
- 10 = Number of site samples
- 10000 = Number of iterations in simulation
- 0.1 = Coefficient of variation of background distribution
- 100 = Mean of background distribution
- 0.05 = Desired level of significance (line included in plots)
- e = Amount of mixture between distributions
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- 20 = Number of background samples
- 20 = Number of site samples
- 10000 = Number of iterations in simulation
- 0.1 = Coefficient of variation of background distribution
- 100 = Mean of background distribution
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- 10 = Number of background samples
- 30 = Number of site samples
- 10000 = Number of iterations in simulation
- 0.1 = Coefficient of variation of background distribution
- 100 = Mean of background distribution
- 0.05 = Desired level of significance (not included in plots)
- e = Amount of mixture between distributions
- Lognormal = Background (and shifted) distribution

The background sample is derived from the indicated distribution with the given mean and coefficient of variation. A second distribution is then defined as a pure shift from the background distribution. It is defined in terms of Pr which measures the probability that a random

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- e = Amount of mixture between distributions
- Lognormal = Background (and shifted) distribution

The background sample is derived from the indicated distribution with the given mean and coefficient of variation. A second distribution is then defined as a pure shift from the background distribution. It is defined in terms of Pr which measures the probability that a random value from the background is less than a random value from the shifted distribution. The site samples are drawn from a mixture of the background and shifted distributions. The proportion of the shifted distribution in the derivation of the site sample mixture distribution is given by the value of epsilon (e).

- 20 = Number of background samples
- 30 = Number of site samples
- 10000 = Number of iterations in simulation
- 0.3 = Coefficient of variation of background distribution
- 100 = Mean of background distribution
- 0.05 = Desired level of significance (line included in plots)
- e = Amount of mixture between distributions
- Lognormal = Background (and shifted) distribution

The background sample is derived from the indicated distribution with the given mean and coefficient of variation. A second distribution is then defined as a pure shift from the background distribution. It is defined in terms of Pr which measures the probability that a random

value from the background is less than a random value from the shifted distribution. The site samples are drawn from a mixture of the background and shifted distributions. The proportion of the shifted distribution in the derivation of the site sample mixture distribution is given by the value of epsilon (e).

- 30 = Number of background samples
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- 100 = Mean of background distribution
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- 10000 = Number of iterations in simulation
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The background sample is derived from the indicated distribution with the given mean and coefficient of variation. A second distribution is then defined as a pure shift from the background distribution. It is defined in terms of P_r which measures the probability that a random

value from the background is less than a random value from the shifted distribution. The site samples are drawn from a mixture of the background and shifted distributions. The proportion of the shifted distribution in the derivation of the site sample mixture distribution is given by the value of epsilon (ϵ).

- 50 = Number of background samples
- 30 = Number of site samples
- 10000 = Number of iterations in simulation
- 0.5 = Coefficient of variation of background distribution
- 100 = Mean of background distribution
- 0.05 = Desired level of significance (line included in plots)
- e = Amount of mixture between distributions
- Lognormal = Background (and shifted) distribution

The background sample is derived from the indicated distribution with the given mean and coefficient of variation. A second distribution is then defined as a pure shift from the background distribution. It is defined in terms of P_r which measures the probability that a random

value from the background is less than a random value from the shifted distribution. The site samples are drawn from a mixture of the background and shifted distributions. The proportion of the shifted distribution in the derivation of the site sample mixture distribution is given by the value of epsilon (e).

- 10 = Number of background samples
- 50 = Number of site samples
- 10000 = Number of iterations in simulation
- 0.5 = Coefficient of variation of background distribution
- 100 = Mean of background distribution
- 0.05 = Desired level of significance (line included in plots)
- e = Amount of mixture between distributions
- Lognormal = Background (and shifted) distribution

The background sample is derived from the indicated distribution with the given mean and coefficient of variation. A second distribution is then defined as a pure shift from the background distribution. It is defined in terms of P_r which measures the probability that a random

value from the background is less than a random value from the shifted distribution. The site samples are drawn from a mixture of the background and shifted distributions. The proportion of the shifted distribution in the derivation of the site sample mixture distribution is given by the value of epsilon (ϵ).

- 20 = Number of background samples
- 50 = Number of site samples
- 10000 = Number of iterations in simulation
- 0.5 = Coefficient of variation of background distribution
- 100 = Mean of background distribution
- 0.05 = Desired level of significance (line included in plots)
- e = Amount of mixture between distributions
- Lognormal = Background (and shifted) distribution

The background sample is derived from the indicated distribution with the given mean and coefficient of variation. A second distribution is then defined as a pure shift from the background distribution. It is defined in terms of P_r which measures the probability that a random

value from the background is less than a random value from the shifted distribution. The site samples are drawn from a mixture of the background and shifted distributions. The proportion of the shifted distribution in the derivation of the site sample mixture distribution is given by the value of epsilon (e).

- 30 = Number of background samples
- 50 = Number of site samples
- 10000 = Number of simulations in simulation
- 0.5 = Coefficient of variation of background distribution
- 100 = Mean of background distribution
- 0.05 = Desired level of significance (line included in plots)
- e = Amount of mixture between distributions
- Lognormal = Background (and shifted) distribution

From the indicated distribution with mean 100 and coefficient of variation 0.5, a second distribution is derived which measures the probability that a random value from the background is less than a random value from the shifted distribution. The site samples are drawn from a mixture of the background and shifted distributions. The proportion of the shifted distribution in the derivation of the site sample mixture distribution is given by the value of epsilon (e).

- 50 = Number of background samples
- 50 = Number of site samples
- 10000 = Number of iterations in simulation
- 0.5 = Coefficient of variation of background distribution
- 100 = Mean of background distribution
- 0.05 = Desired level of significance (line included in plots)
- e = Amount of mixture between distributions
- Lognormal = Background (and shifted) distribution

The background sample is derived from the indicated distribution with the given mean and coefficient of variation. A second distribution is then defined as a pure shift from the background distribution. It is defined in terms of Pr which measures the probability that a random

value from the background is less than a random value from the shifted distribution. The site samples are drawn from a mixture of the background and shifted distributions. The proportion of the shifted distribution in the derivation of the site sample mixture distribution is given by the value of e .

- 50 = Number of background samples
- 50 = Number of site samples
- 10000 = Number of iterations in simulation
- 0.5 = Coefficient of variation of background distribution
- 100 = Mean of background distribution
- 0.05 = Desired level of significance (line included in plots)
- e = Amount of mixture between distributions
- Lognormal = Background (and shifted) distribution

The background sample is derived from the indicated distribution with the given mean and coefficient of variation. A second distribution is then defined as a pure shift from the background distribution. It is defined in terms of Pr which measures the probability that a random

value from the background is less than a random value from the shifted distribution. The site samples are drawn from a mixture of the background and shifted distributions. The proportion of the shifted distribution in the derivation of the site sample mixture distribution is given by the value of e .

- 10 = Number of background samples
- 10 = Number of site samples
- 10000 = Number of iterations in simulation
- 0.7 = Coefficient of variation of background distribution
- 100 = Mean of background distribution
- 0.05 = Desired level of significance (line included in plots)
- e = Amount of mixture between distributions
- Lognormal = Background (and shifted) distribution

The background sample is derived from the indicated distribution with the given mean and coefficient of variation. A second distribution is then defined as a pure shift from the background distribution. It is defined in terms of P_r which measures the probability that a random

value from the background is less than a random value from the shifted distribution. The site samples are drawn from a mixture of the background and shifted distributions. The proportion of the shifted distribution in the derivation of the site sample mixture distribution is given by the value of epsilon (e).

- 20 = Number of background samples
- 10 = Number of site samples
- 10000 = Number of iterations in simulation
- 0.7 = Coefficient of variation of background distribution
- 100 = Mean of background distribution
- 0.05 = Desired level of significance (line included in plots)
- e = Amount of mixture between distributions
- Lognormal = Background (and shifted) distribution

The background sample is derived from the indicated distribution with the given mean and coefficient of variation. A second distribution is then defined as a pure shift from the background distribution. It is defined in terms of Pr which measures the probability that a random

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- 30 = Number of background samples
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- 10000 = Number of iterations in simulation
- 0.7 = Coefficient of variation of background distribution
- 100 = Mean of background distribution
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- 10 = Number of background samples
- 10 = Number of site samples
- 10000 = Number of iterations in simulation
- 1.0 = Coefficient of variation of background distribution
- 100 = Mean of background distribution
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- e = Amount of mixture between distributions
- Lognormal = Background (and shifted) distribution

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value from the background is less than a random value from the shifted distribution. The site samples are drawn from a mixture of the background and shifted distributions. The proportion of the shifted distribution in the derivation of the site sample mixture distribution is given by the value of epsilon (e).

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ATTACHMENT B**Power Curve Plots of Monte Carlo Simulations for the State and the WQH tests,
Using a Weibull Distribution.****EXPLANATION**

The plots contained in this attachment compare the performance of the State and WQH tests for a range of conditions, as described in the text. In all of the plots, the x-axis (abscissa) is the probability of exceedance (P_r), and the y-axis (ordinate) is the probability that the test indicates that the site is contaminated.

- 10 = Number of background samples
- 10 = Number of site samples
- 10000 = Number of iterations in simulation
- 0.1 = Coefficient of variation of background distribution
- 100 = Mean of background distribution
- 0.05 = Desired level of significance (line included in plots)
- e = Amount of mixture between distributions
- Weibull = Background (and shifted) distribution

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value from the background is less than a random value from the shifted distribution. The site samples are drawn from a mixture of the background and shifted distributions. The proportion of the shifted distribution in the derivation of the site sample mixture distribution is given by the value of e .

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value from the background is less than a random value from the shifted distribution. The site samples are drawn from a mixture of the background and shifted distributions. The proportion of the shifted distribution in the derivation of the site sample mixture distribution is given by the value of epsilon (e).

- 20 = Number of background samples
- 30 = Number of site samples
- 10000 = Number of iterations in simulation
- 0.3 = Coefficient of variation of background distribution
- 100 = Mean of background distribution
- 0.05 = Desired level of significance (line included in plots)
- e = Amount of mixture between distributions
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- 10 = Number of background samples
- 10 = Number of site samples
- 10000 = Number of iterations in simulation
- 0.7 = Coefficient of variation of background distribution
- 100 = Mean of background distribution
- 0.05 = Desired level of significance (line included in plots)
- e = Amount of mixture between distributions
- Weibull = Background (and shifted) distribution

The background sample is derived from the indicated distribution with the given mean and coefficient of variation. A second distribution is then defined as a pure shift from the background distribution. It is defined in terms of P_r which measures the probability that a random

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- 1.0 = Coefficient of variation of background distribution
- 100 = Mean of background distribution
- 0.05 = Desired level of significance (line included in plots)
- e = Amount of mixture between distributions
- Weibull = Background (and shifted) distribution

The background sample is derived from the indicated distribution with the given mean and coefficient of variation. A second distribution is then defined as a pure shift from the background distribution. It is defined in terms of Pr which measures the probability that a random

value from the background is less than a random value from the shifted distribution. The site samples are drawn from a mixture of the background and shifted distributions. The proportion of the shifted distribution in the derivation of the site sample mixture distribution is given by the value of epsilon (e).

- 30 = Number of background samples
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