GROUNDWATER STATISTICS TOOL

USER'S GUIDE

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1.0 BACKGROUND/PURPOSE

The Groundwater Statistics Tool is designed to help evaluate contaminant of concern (COC) concentrations on a well-by-well basis to determine whether a groundwater restoration remedial action is complete. The tool is designed to support the U.S. Environmental Protection Agency (EPA) memorandum, "Guidance for Evaluating Completion of Groundwater Restoration Remedial Actions" (EPA 2013b, referred to as the *Groundwater Restoration Completion Guidance*), and comports with principles outlined in the "Recommended Approach for Evaluating Completion of Groundwater Restoration Remedial Actions at a Groundwater Monitoring Well" (EPA 2014, referred to as the *Recommended Approach*). Both of these guidance documents should be reviewed before using the tool.

The tool is a Microsoft Excel workbook that is intended to evaluate data for a single COC at a single well. Each Excel worksheet ("screen") is protected to prevent accidental overwriting of formulas. The tool was developed in Excel 2010; using an older version of Excel or a version using personal computer (PC) emulation in a non-PC environment may not allow use of all of the tool's capabilities. The tool should generally be run separately for each well and each COC being evaluated.

There are two phases of the groundwater restoration process that the tool is designed to evaluate: the remediation monitoring phase, and attainment monitoring phase.

1.1 Remediation Monitoring Phase

The following text from the *Recommended Approach* discusses the remediation monitoring phase:

> "As discussed in the Groundwater Restoration Completion Guidance, the remediation monitoring phase refers to the phase of the remedy where either active or passive remedial activities are being implemented to reach groundwater cleanup levels selected in a decision document. During this phase, groundwater sampling and monitoring data typically are collected to evaluate contaminant migration and changes in COC concentrations over time. The completion of this phase typically provides stakeholders a decision point for starting data collection and evaluation of the attainment monitoring phase. If an active treatment system is being employed at the site, the completion of this phase may also provide stakeholders with an opportunity to evaluate terminating the system, as appropriate, in the vicinity of the well or wells where groundwater restoration completion is being evaluated. If passive systems are being employed at the site, the data used to make the remediation phase completion conclusion may also be useful as part of the attainment phase evaluation since active systems are not being employed.
>
> The remediation phase at a monitoring well typically is completed when the data collected and evaluated demonstrate that the groundwater has reached the cleanup levels for all COCs set forth in the record of decision (ROD). It is important to note that at any time during the groundwater remediation, conclusions may be made to remove certain COCs from the monitoring program based on their COC-specific trends or presence in the well. If certain

COCs are no longer being evaluated in a well, the rationale for discontinuing monitoring may be used, in conjunction with the current well data, to make the conclusion that all COCs have reached their cleanup levels."

The user should note the following considerations regarding data requirements for each well and COC:

- EPA guidance (2014) recommends a minimum of four data points to evaluate completion of this phase. In addition, the tool requires a minimum of four detected results to complete statistical calculations because upper confidence limit (UCL) and trend calculations require at least four detected results to be reliable.
- EPA guidance (2014) provides the user with an option to use a trend test or a mean test on the remediation monitoring phase data set. In this situation, the selection of the best statistical tool is based on the user and best professional judgment.
    - Trend test: The time-dependent trend line is calculated for this test. It is recommended that the trend test generally be used for a data set that has a protracted steep change in concentration over time with data points that cross below the cleanup level. A less steep change (or asymptotic condition) may not lend itself to a trend test. Once the trend is calculated, an upper confidence band on the trend line should be calculated to allow the user to account for variability within the data set. The use of the upper confidence band on the trend line accounts for uncertainty and provides confidence that the COC cleanup level has been achieved. In general, a 95 percent confidence level is recommended for calculating the upper confidence band.
    - Mean test: It is recommended that the mean test generally be used for the data set that does not have a steep change in concentration over time. A steep change would provide high variability in the data set and would tend to elevate the UCL on the mean. Statistics are used to determine the mean contaminant concentration from these data for the COC for this test. The UCL is calculated once the mean is established. The UCL should be compared against the cleanup level. The use of the UCL value accounts for uncertainty and provides confidence that the COC cleanup level has been achieved. In general, the 95 percent UCL is used as the recommended confidence limit.

1.2 Attainment Monitoring Phase

The following text from the *Recommended Approach* discusses the attainment monitoring phase:

"The attainment monitoring phase typically occurs after a Region makes a determination that the remediation monitoring phase is complete. When the attainment monitoring phase begins, data typically are collected to first evaluate whether the well has reached steady-state conditions where active remediation activities, if employed, are no longer influencing the groundwater in the well. Once the groundwater is observed to have reached steady-

state conditions, data should be collected and evaluated to confirm the attainment monitoring phase has been completed."

The attainment monitoring phase at a monitoring well typically is complete when contaminant-specific data provide a technical and scientific basis that:

(1) The contaminant cleanup level for each COC has been achieved; and

(2) The groundwater will continue to meet the contaminant cleanup level for each COC in the future.

The user should note the following considerations regarding data requirements:

- EPA guidance (2014) recommends a minimum of eight data points generally be used to evaluate completion of this phase. However, the tool requires a minimum of four data points to run the attainment monitoring phase calculations to accommodate site-specific cases. In addition, the tool requires a minimum of four detected results to complete statistical calculations because UCL and trend calculations require at least four detected results to be reliable.
- EPA guidance (2014) recommends evaluating data to determine whether steady-state conditions have been reached for a COC in a well. If steady-state conditions have been reached, it may be appropriate to include some of the remediation monitoring phase data points in the data set used to evaluate the attainment monitoring phase.
- EPA guidance (2014) recommends evaluating the attainment monitoring phase by applying both the UCL on the mean and the trend test.
    - UCL on the mean: Statistics are used for this test to determine the mean contaminant concentration from the data for the COC. The UCL is calculated once the mean is established. The UCL should be compared with the cleanup level. Using the UCL value accounts for uncertainty and provides confidence that the COC cleanup level has been achieved. In general, the 95 percent UCL is used as the recommended confidence limit.
    - Trend: Statistics are used to determine the time-dependent trend line for this test. The slope of the trend line is used to make a conclusion on future groundwater conditions. If the trend line has a statistically significant zero or negative slope (indicating steady-state conditions or decreasing concentrations), it may be appropriate to conclude that the contaminant concentrations for each COC in groundwater will remain at or below the cleanup level.

2.0 OVERVIEW OF THE GROUNDWATER STATISTICS TOOL

The tool is designed to provide a statistical evaluation of a data set to determine that the expectations outlined in EPA guidance (2013b and 2014) and outlined above in this User's Guide have been achieved. In addition to providing statistical mean, trend, and UCL calculations, the tool also tests for detection frequency, outliers, and normality. These tests are described in the following sub-sections. Most of the statistical tests used in the tool are based on the "Unified Guidance for Statistical Analysis of Groundwater Monitoring Data at RCRA Facilities," which will be referred to as the *Unified Guidance* (EPA 2009).

2.1 Outlier Testing

Outliers are checked with a Dixon's test, which is appropriate for data sets composed of fewer than 25 samples. For more details on outliers and the mechanics of the Dixon's test, see Section 12.3 of the *Unified Guidance* (EPA 2009). A confidence level of 1 percent is recommended for the Dixon's test and is established as the default in cell A19 of the Data Input screen. However, alternative confidence levels for the test can be specified (10 percent, 5 percent, or 0.5 percent). Dixon's test is used only to indicate whether a data point can be considered as an outlier statistically; outliers should not be discarded from the data set unless there is also a valid, known technical reason for the outlier.

2.2 Normality Testing

The normality of the data set is checked using a Shapiro-Wilk test. For details on normality and the mechanics of the Shapiro-Wilk test, see Section 10.5 of the *Unified Guidance* (EPA 2009). Different levels of confidence are used based on the size of the data set (n=number of samples in data set):

- $n < 10$ – use a confidence level of 10 percent
- $10 \leq n < 20$ – use a confidence level of 5 percent
- $n \geq 20$ – use a confidence level of 1 percent

2.3 Calculations of the Mean, Linear Trend and Upper Confidence Band

A confidence level of 95 percent is recommended for the mean calculations and represents the common practice for calculating the UCL on the mean. As shown in Table 1, the UCL on the mean is calculated in different ways, depending on the characteristics of the data set.

A confidence level of 95 percent is recommended to calculate confidence around a trend line and represents the common practice for this calculation. The linear trend and upper confidence band are calculated in different ways, depending on the characteristics of the data set, as shown in Table 2.

Table 1. Methods for Calculating UCLs on the Mean by Data Set Type

Detection Frequency	Type of Data Set (Based on Shapiro-Wilk Test of Data)	
	Normal	Nonparametric
DF = 100%	Student's-t UCL	Chebyshev UCL
0% < DF < 100%	KM Chebyshev UCL	KM Chebyshev UCL
0%	No UCL is calculated	No UCL is calculated

Notes:
KM Kaplan-Meier
DF Detection frequency
UCL Upper confidence limit

Table 2. Methods for Calculating Linear Trends and Confidence Bands by Data Set Type

Detection Frequency	Type of Data Set (Based on Shapiro-Wilk Test on Residuals)	
	Linear	Nonlinear
DF = 100%	Linear Regression	Theil-Sen line, Mann-Kendall test
0% < DF < 100%	Linear Regression*	Theil-Sen line, Mann-Kendall test
0%	No trend is calculated	No trend is calculated

Notes:
* Before the linear regression is calculated, each nondetect result is substituted with a randomly generated real number between zero and the reported detection limit. This substitution prevents the introduction of artificially low variability from multiple identical (or similar) detection limits.
DF Detection frequency

2.4 Data Sets with No Detected Values

As noted in Tables 1 and 2, the tool will not calculate a UCL on the mean, a trend line, or an upper confidence band if none of the concentrations are above the detection limit. In this situation, the project team can generally conclude that the phase being evaluated is complete by visual, or a non-statistical, evaluation if the detection limits for non-detects in the data set are below the contaminant cleanup level.

3.0 STEP-BY-STEP INSTRUCTIONS FOR USING THE GROUNDWATER STATISTICS TOOL

This tool takes the user through one data input and four results screens. Each screen is protected to prevent accidental overwriting of formulas. These screens are:

1. The "Data_Input" screen.
2. The "Outliers" screen.
3. The "Normality" screen.
4. The "Trend" screen.
5. The "UCL" screen.

In addition to the data input and results screens, the tool provides a screen titled "Example Data." This screen provides several synthesized data sets that illustrate various functions of the tool. These example data sets are discussed in the Examples section. Example data sets 5 through 9 can document the tool's performance compared with example results calculated in the *Unified Guidance*.

Step 1: On the "Data_Input" screen, enter descriptive data into cells B4 to B21, D7 to F26, and I24 to L24. Descriptive data capture information to describe the site, the monitoring phase being evaluated, the COC, and related information that describe the site and purpose of the evaluation. The cells for entering descriptive data are color-coded green; cells in blue are locked and show outputs that the user cannot alter. Control buttons are located in cells that are color-coded red; use these control buttons to move forward and backward through the tool. Follow the instructions below for data entry:

a. Enter the name of the site in cell B4. No restrictions.

b. Enter the operating unit (OU) in cell B5 (if applicable). No restrictions.

c. Select the type of evaluation in cell B6. This value should be either "Remediation" or "Attainment," and there is a drop-down menu to aid in the selection.

d. Enter the date of the evaluation in cell B7. There are no restrictions on how the date is entered. Examples include: March 1, 2014, 3/1/2014, 3/1/14, March 2014.

e. Enter the name of the person performing the evaluation in cell B8. No restrictions.

f. Enter the COC in cell B10. No restrictions.

g. Enter the well name or number in cell B11. No restrictions.

h. Enter the units for date in cell B12. This value should be "Day," "Month," "Year," or "Date," and there is a drop-down menu to aid in the selection. The entries are expected to be dates, or may be days, months, or years from a starting value (which may be zero). If cell B12 is set to some value other than "Date" when dates have already been entered into the data entry table in column D, the values will be displayed as large integer values because of the way Excel handles dates.

i. Enter the units for concentration in cell B13. No restrictions. These units should be the same as the units for the cleanup level in cell B16.

j. Enter the confidence level desired in cell B15 using the drop-down menu to aid in the selection. The default is the recommended confidence level of 95 percent.

k. Enter the cleanup level for the COC in cell B16. This value should be a positive real number and should be extracted from the remedy decision document.

l. Enter the type of cleanup level being compared in cell B17/B18 (for example, Maximum Contaminant Level [MCL] or risk-based concentration). No restrictions. The type of cleanup level should be extracted from the remedy decision document.

m. Enter the risk of false outlier rejection in cell B19. This value should be "0.5%," "1%," "5%," or "10%," and there is a drop-down menu to aid in the selection. The default is 1 percent. Selecting a higher value increases the likelihood that a data point may be falsely flagged as a potential outlier; selecting a lower value decreases this likelihood.

n. **Random Seed:** Cell B20 is a placeholder for a random seed. The random seed is used to calculate imputed values for non-detect data points. The random seed is also used to calculate the time-dependent upper confidence band for nonparametric data sets using a bootstrap procedure. In general, the user should leave this value blank when the data are initially entered. If non-detects are present in the data set or if it is determined that the data set in nonparametric, the tool will automatically generate a random seed. Since the random seed is generated off an internal clock, the value (assuming nothing is entered during data entry) will be different each time the tool is run. After a data set analysis is conducted, the user should document the random seed value. Documenting this value will allow the results to be replicated. If you desire to replicate results, you may enter this random seed value (a positive real number) in cell B20 for subsequent data calculations.

o. Enter the number of significant figures to use for reporting UCLs and predicted concentrations in cell B21. This value should be a positive whole number greater than zero. The tool restricts the number of significant figures to be between 1 and 3, since analytical precision is not expected to exceed three significant figures. The default value is 2. A drop-down menu is provided to assist with the selection.

p. Time and concentration data may be entered manually into the data entry table in cells D7 to F26 using the keyboard; however, the preferred method is to enter data by copying and pasting from another Excel spreadsheet (as long as the organization is the same and only the three columns, D through F, are pasted into the data entry table) to reduce input error. Excel's "paste values" method can be used to avoid overwriting the formatting of the cells.

   The tool's data entry table is set up for a maximum of 20 data points. If more than 20 data points are available, it is recommended that only the most recent 20 be used. If the user wants to conduct a trend analysis of more than 20 data points, other software tools such as ProUCL (EPA 2013a) or MAROS (AFCEE 2006) can be used.

1. Enter the measurement dates in column D between rows 7 to 26. These dates are expected to be actual dates, or may be days, months, or years from a starting value (which may be zero). A few notes regarding the data set:
    i. The type of date input (day, month, or actual date) should be consistent throughout the data set. This allows for accurate trend analysis.
    ii. All data should be entered in increasing chronological order (oldest to newest).
    iii. If duplicate data are available for a specific date, only one data entry for that date should be made.
2. Enter the measured concentrations in column E between rows 7 and 26. These values are restricted to real numbers greater than zero.
    i. If the date corresponds to a duplicate sampling event, it is recommended that the user enter either the maximum concentration or the average concentration in the concentration field, as agreed by the project team.
    ii. If the measurement is categorized as a non-detect, it is recommended that the user enter the reporting limit for the analytical method. **The user should NOT enter zero or an arbitrary number.**
3. Enter the data qualifier in column F between rows 7 and 26. Use either "U" or "ND" for undetected or nondetected results. Based on the qualifier, column G will be populated with a "yes" or "no" to indicate whether the concentration is a detected result (for a "yes") or a detection limit for a nondetected result (for a "no"). Blank cells are allowed, and qualifiers do not need to be entered if they are not applicable.

q. In cells I24 to L24, enter the minimum and maximum values for the date and concentration axes of plots shown on the various reports. The default selection is "Auto," which will use Excel's automatic setting for the charts. Adjusting these values can make the data plots easier to view.

Step 2: Review the Data Review and Recommendations section at the bottom of the "Data_Input" screen. If no recommendations appear in red text, the data are ready for statistical analysis. If recommendations appear in red text, the user should follow the recommendations before proceeding with the statistical analysis. Although the statistical analysis can be run without addressing the recommendations, error messages will result.

Step 3: Click the button labeled "Next Step: Check for Outliers." The tool will run Dixon tests to check for outliers and will display the results of the tests on the "Outliers" screen.

a. Rows 5 and 6 show the number of data points and the selected risk of false rejection, both of which were previously entered on the "Data_Input" screen.

b. Row 7 shows the critical value used for the Dixon's test, which is based on the number of data points and the selected risk of false rejection.

c. Row 8 shows the outlier type being tested. Both low concentration (column B) and high concentration (column C) outliers are tested.

d. Row 9 shows the test statistic. For details on how the test statistic is calculated, refer to Section 12.3 of the *Unified Guidance* (EPA 2009). The test statistic is compared with the critical value to determine whether the lowest concentration data point is a potential low outlier or the highest concentration data point is a potential high outlier.

e. Row 10 shows the result of the test. "Yes" is displayed if a potential outlier is indicated; otherwise "No" is displayed.

f. Row 11 uses the results of the normality testing (which will be shown on the next screen) to indicate whether the Dixon's test is valid. Since Dixon's test requires that the data are normally distributed, the test is not valid and should not be used to justify an outlier when the data are not normally distributed. Nonparametric outlier tests may be used, but these tests are not included in this tool.

g. If row 10 of the "Outliers" screen indicates no potential outliers, the user may proceed by clicking the button labeled "Next Step: Normality Screen."

h. If row 10 of the "Outliers" screen indicates that potential outliers are present in the data set and row 11 indicates that the Dixon's test is valid for that potential outlier, the user may want to consider revising the data set to remove the outlier. Outliers should be removed only if a valid technical reason for the outlier is known and the project team or user concludes an acceptable reason exists to remove the outlier. There are two options for proceeding in the presence of an outlier:

    i. Elect to remove the outlier. The outlier can be removed from the data set in one of two ways: 1) click the button labeled "Previous Step: Data Input Screen" to return to the "Data Input" screen or 2) click the button labeled "Next Step: Normality Screen", where a pop up box will be displayed. To get back to the "Data Input" screen, a "N" should be entered in the prompt.

    Upon returning to the "Data Input" screen to remove the outlier(s) from the data set, the user should first delete the "date" (column D) and "concentration" (column E) values for the outlier(s). The user should then "Copy" the date and concentration values for all data that was collected chronologically after the outlier(s). The user should then paste the copied cells into the table starting in the row where the original outlier(s) was deleted. The user should then delete the data in the final row(s) to ensure there is no duplicative data in the set (however, the entire row should not be deleted).

    Note: When modifying the data set, do not use the "Cut" function.

    ii. Retain full data set. If the user elects to retain the outlier(s) and move forward with the statistical analysis, the user should click the button labeled "Next Step: Normality Screen" and enter "Y" into the prompt field.

Step 4: The tool will run three Shapiro-Wilk tests on the data set to determine whether the data and the residuals appear to be normally distributed. The three test results are shown on the "Normality" screen. The first column is for the full data set and is used to determine which UCL calculation method (normal or nonparametric) should be used. The second column is for the data set minus the potential outliers and is used only to determine whether the Dixon test is valid. Dixon's test is not considered valid if the data set minus the potential outliers does not appear to be normal. If no outliers exist, the column for the data set minus potential outliers will not be populated with results. The third column is for the residuals and is used to test whether parametric or non-parametric methods are used for fitting the trend. The following results are shown for each test:

a. Rows 7 and 8 show the number of data points and the selected alpha values for the Shapiro-Wilk test. The number of data points was previously calculated in cell B23 on the "Data_Input" screen. The alpha value for the Shapiro-Wilk test is equal to 100 percent minus the confidence level previously entered in cell B15 on the "Data_Input" screen.

b. Rows 9, 10 and 11 show the slopes, intercepts and correlation coefficients (R) of the normal Q-Q plot. These are shown for informational purposes only.

c. Row 12 shows the exact Shapiro-Wilk test values. For more detail on how the test value is calculated, see Section 10.5 of the *Unified Guidance* (EPA 2009).

d. Row 13 shows the critical values for each test, which is based on the number of data points and the Shapiro-Wilk alpha values. For more detail on how the critical value is determined, see Section 10.5 of the *Unified Guidance* (EPA 2009).

e. Row 14 shows the result of the tests. If the exact test value is lower than the critical value, the conclusion of the test is that the data (or the residuals, for the third column) do not appear normal. If the exact test value is equal to or greater than the critical value, the conclusion of the test is that the data (or the residuals, for the third column) appear normal.

The user may now proceed to either the "Trend" screen, the "UCL" screen or return to the "Outliers" screen by using the buttons at the bottom of the screen.

An error message will appear if the trend predicts negative concentrations during the time period of the measurements entered into the tool. In this case, the message will inform the user that the data set cannot be evaluated by the tool. This situation can occur when there is a steep trend in the data that ends (or starts) near a concentration of zero. This situation is not expected to occur commonly; if it does occur, there are two ways to correct the situation.

1. Data points can be removed from the data set. Often, a case may be observed where a group of data points within the data set has a steeply decreasing trend and these data points are followed by a group of data points with a less steep trend, In this case, the early points where the concentration is decreasing rapidly should be removed, while the number of data points recommended for the decision (as described in Section 1) is maintained. Data points at the end of the data set should <u>not</u> be removed.

2. Normalizing transformations of the data may be attempted to account for the change in slope. This tool (or another tool such as ProUCL [EPA 2013a]) may still be used for trend testing, but the data must be transformed outside the tool and imported into the tool. For example, the logarithms of the concentration can be calculated and imported into the tool to perform a logarithmic transformation. The user may want to consult a statistician for assistance with this process. In this situation, the UCL must be calculated on the untransformed data; only the trend should be calculated using the transformed data. For more details on other transformations that can be attempted with the data, see Section 3.2.4 of the *Unified Guidance* (EPA 2009).

Step 5: Inspect the results on the "Trend" screen.

- If the trend is found to be linear, the trend will be evaluated using the ordinary least squares method. The following outputs will be shown:
    - The data set will be shown in columns B and C of the table. The predicted concentrations from the ordinary least squares method, the residuals (difference between the measured and predicted concentrations), and the calculated values of the 95 upper confidence band for each data point will also be shown in columns D, E, and F of the table.
    - The slope, intercept and R-squared values of the linear regression trend line will be shown in cells I7, I8, and I9.
    - The test statistic will be shown in cell I11. For details on calculation of the test statistic, see Section 17.3.1 of the *Unified Guidance* (EPA 2009).
    - The critical value of the test will be shown in cell I12. The critical value is based on the number of data points and the confidence level selected on the "Data Input" screen, and will have the same sign as the slope.
    - The test result will be shown in cell I10. If the critical value is positive and the test statistic is greater than the critical value, the conclusion is that the trend is increasing; otherwise, the conclusion is that there is no trend. If the critical value is negative and the test statistic is lower than the critical value, the conclusion is that the trend is decreasing; otherwise, the conclusion is that there is no trend.
    - If the trend is increasing, the date at which the concentration is predicted to exceed the cleanup level is shown in cell I13. If the trend is not increasing, the message "Not applicable – slope is not statistically increasing" will be displayed.
- If the trend is not found to be linear, the trend will be evaluated using the Mann-Kendal test using a Theil-Sen slope. The following outputs will be shown:
    - The data set will be shown in columns B and C of the table. The predicted concentrations from the ordinary least squares method, the residuals (difference between the measured and predicted concentrations), and the calculated values of the upper confidence band for each data point will also be shown in columns D, E, and F of the table.

  - The critical value of the test will be shown in cell I12. The critical value is based on the number of data points and the confidence level selected on the "Data Input" screen and will have the same sign as the slope.
  - The test statistic and normalized S value will be shown in cells I8 and I9. For details on the calculation of these values, see Section 17.3.2 of the *Unified Guidance* (EPA 2009).
  - The slope and intercept of the Theil-Sen trend line will be shown in cells L7 and L8.
  - If the trend is increasing, the date at which the concentration is predicted to exceed the cleanup level is shown in cell L9. If the trend is not increasing, the message "Not applicable – slope is not statistically increasing" will be displayed.
- The trend line is displayed on a plot. The confidence band on the trend will also be displayed.

The user may now proceed to the "UCL" screen.

Step 6: Inspect the results on the "UCL" screen. The screen shows the calculated UCL, the value of the upper confidence band at the final sampling event, and the result of the trend calculations. It also includes a summary of the data entered on the "Data_Input" screen and shows the appropriate trend information. If nondetects are present, the tool displays a table that summarizes the data and the imputed values assigned by the tool.

4.0 EXAMPLES

As noted earlier, several example data sets are provided on the "Example Data" screen. Each data set is discussed briefly in the sections below. The last eight examples are not meant specifically to test the remediation and attainment decisions, although a decision will be shown on the "UCL" screens based on the settings for the decision type, cleanup level, and confidence levels. For Examples 5 through 9 from (), the corresponding results in the *Unified Guidance* (EPA 2009) may differ slightly from the results calculated by the tool because of differences in rounding. Figures at the end of this guide show screenshots for Examples 1 through 4.

- Example Data Set 1. This data set is for trichloroethene and consists of eight data points. These data are for the remediation monitoring phase at a 95 percent confidence level. There are two sub-examples here:
    - If all eight points are used, the data set is not normally distributed and the residuals are not normally distributed; therefore, the 95 percent UCL and trends will be calculated using nonparametric methods. The 95 percent upper confidence band at the final sampling event is found to be below the cleanup level (MCL of 5 parts per billion [ppb]), but the fit to the data results in predictions of negative concentrations, and an error message is generated when the user clicks the "Next Step: Trend Screen" on the "Normality" screen. Screen shots of the "Data_Input" and "Normality" screens for this case are shown in Figures 1 and 2.
    - If only the last four data points are used, where the data are closer to the MCL and more linear, the 95 percent upper confidence band at the final sampling event will be below the MCL, and no negative concentrations are predicted. Although the overall 95 percent UCL of the data set is above the MCL, only one criterion must be met to proceed to attainment. Screen shots of the "Data," Outlier," "Normality," "Trend," and "UCL" screens for this case are shown in Figures 3 through 7.
- Example Data Set 2. This data set is a continuation of the previous data set for trichloroethene and consists of 10 data points for the attainment monitoring phase. Again, there are two sub-examples here:
    - If only the first eight points are used, the data set is found to have a statistically significant decreasing trend, but the calculated 95 percent UCL is not below the MCL. Screen shots of the "Data" and "UCL" screens for this case are shown in Figures 8 and 9.
    - If all 10 data points are used, the data set is found to satisfy both attainment criteria identified in Section 1.2; the trend is statistically significant and decreasing, and the 95 percent UCL is below the MCL. In fact, this scenario is also the case after nine sampling events. Screen shots of the "Data" and "UCL" screens for this case are shown in Figures 10 and 11.

- Example Data Set 3. This data set is for vinyl chloride at the same hypothetical site as for examples 1 and 2 and is for the remediation monitoring phase. The concentration is observed to be increasing toward the MCL and there is a slight elevated result at the seventh event. Although the upper confidence band exceeds the MCL of 2 ppb, the 95 percent UCL does not. Only one criterion must be met to proceed to attainment, so the remediation monitoring phase is considered complete. Screen shots of the "Data" and "UCL" screens for this case are shown in Figures 12 and 13.
- Example Data Set 4. This data set is a continuation of the previous data set for vinyl chloride and consists of 10 data points for the attainment monitoring phase. The first two data points are the last two from the remediation monitoring phase, which is consistent with the "Recommended Approach" (EPA 2014). Although all 10 points could be used, both the UCL and slope criteria for the attainment monitoring phase are met if only the first eight are used. Screen shots of the "Data" and "UCL" screens for this case are shown in Figures 14 and 15.
- Example Data Set 5. This data set is Example 12-3 from Section 12.3 of the *Unified Guidance* (EPA 2009). The data are the logged concentrations from the example. There are 20 data points, and the 20^{th} data point is an outlier at the 95 percent confidence level. Additional calculations can be examined for this example, but it is intended to illustrate the tool's use in checking the outlier calculations.
- Example Data Set 6. This data set is modified from the previous data set by subtracting each concentration from 10 ppb. There are 20 data points, and the 20^{th} data point is an outlier at the 95 percent confidence level. Additional calculations can be examined for this example, but it is intended for use in checking the outlier calculations.
- Example Data Set 7. This data set is from Example 10-2 in Section 10.5.1 of the *Unified Guidance* (EPA 2009). The data set has 20 data points and is not normal at the 99 percent confidence level. The example can be checked by proceeding to the "Normality" screen and comparing the test results against the example in the *Unified Guidance*. Additional calculations can be examined for this example, but it is intended for use in checking the normality calculations. If trend or UCL calculations are attempted, this example will generate an error message because negative concentrations are predicted for the early data points.
- Example Data Set 8. This data set is from Example 17-5 in Section 17.3.1 of the *Unified Guidance* (EPA 2009). The data set has 19 data points with normal residuals. It can be used to illustrate the linear regression and compare it against the results for the example in the *Unified Guidance*. The trend is shown to be statistically increasing at the 99 percent confidence level in the example.
- Example Data Set 9. This data set is from Example 21-7 in Section 21.3.1 of the *Unified Guidance* (EPA 2009). The data set has 10 data points, with normal residuals. It can be used to illustrate both the linear regression and the upper confidence band calculations and compare them against the example. The upper confidence band is calculated at the 95 percent confidence level in the example.

- Example Data Set 10. This data set is the same as example data set 9, described above, with one change. One additional result is added, a nondetect at a detection limit of 2 ppb. This data set can be used to illustrate UCLs calculated based on the nonparametric Kaplan-Meier (KM) Chebyshev UCL. In this example, the residuals are still normal, so the trend will be calculated using linear regression but using an imputed value for the nondetect result. If a system-generated random seed predicts negative concentrations, use a random seed of 62311.421888.
- Example Data Set 11. This data set is the same as example data set 9, described above, with changes. The last two results are changed to nondetect results with a detection limit of 15 ppb, and three additional identical results are added. This data set can be used to illustrate UCLs calculated based on the nonparametric KM Chebyshev UCL. In this example, the residuals are not normal, so the trend will be calculated using the Theil-Sen option with a Mann-Kendall test for statistical significance. If a system-generated random seed predicts negative concentrations, use a random seed of 62311.421888.
- Example Data Set 12. This data set is based on Example 21-8 in Section 21.3.2 of the *Unified Guidance* (EPA 2009). The data set has 10 data points, with normal residuals; the final data point has been altered from the original example so that the trend is not statistically significant at the 95 percent confidence level; this data set illustrates how the output will appear if the trend is not found to be statistically significant.

5.0 REFERENCES

Air Force Center for Environmental Excellence (AFCEE). 2006. Monitoring and Remediation Optimization Systems (MAROS) Software Version 2.2 User Guide. March.

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EPA. 2013a. ProUCL Version 5.0.00 Technical Guide, Statistical Software for Environmental Applications for Data Sets with and without Nondetect Observations. September.

EPA. 2013b. Guidance for Evaluating Completion of Groundwater Restoration Remedial Actions. OSWER 9355.0-129. From: James E. Woolford, Director, Office of Superfund Remediation and Technology Innovation; and Reggie Cheatham, Director, Federal Facilities Restoration and Reuse Office. To: Superfund National Policy Managers, Regions 1 - 10; and Federal Facility Leadership Council. November 25.

EPA. 2014. Recommended Approach for Evaluating Completion of Groundwater Restoration Remedial Actions at a Groundwater Monitoring Well. OSWER 9283.1-44. Draft.

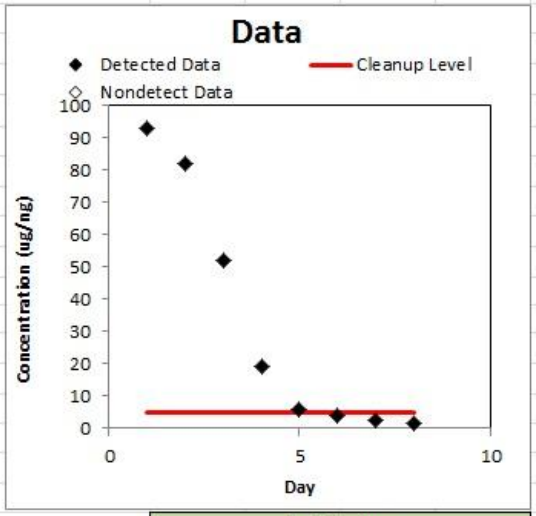
Figure 1. Data Input Screen for Trichloroethene Remediation Example 1, All Eight Data Points Used

Groundwater Statistics Tool

Data input worksheet

Site Name	Test
Operating Unit (OU)	Test
Type of Evaluation	Remediation
Date of Evaluation	6/11/2014
Person performing analysis	RT
Chemical of Concern	TCE
Well Name/Number	1
Date Units	Month
Concentration Units	ug/L
Confidence Level Desired	95%
Cleanup Level	5
Source of cleanup level (e.g. MCL or risk-based concentration)	MCL
Risk of False Outlier Rejection	1%
Random Seed (may be left blank)	62311.42188
Significant figures to use	3
Number of data points:	8
Number of detected results:	8
Number of nondetect results:	0
Detection frequency:	100%

Date (Month)	TCE Concentration (ug/L)	Data Qualifier	Detected? (Yes or No)
1	93		Yes
2	82		Yes
3	52		Yes
4	19		Yes
5	6.1		Yes
6	4.2		Yes
7	2.8		Yes
8	1.8		Yes



Axis Values			
Time		Concentration	
Min	Max	Min	Max
Auto	Auto	Auto	Auto

Reset Concentration Axis

Data Review		Recommendations
Are all necessary data fields entered, and in proper format?	Yes	None
Are at least 4 data points present for statistical analysis?	Yes	None
Are detection limits for nondetects ≤ maximum detected value?	Yes	None
Are all data within chart axis limits?	Yes	None

Pressing the "Check for Outliers" button to the right will open a worksheet that shows the results of a Dixons's test for outliers.

Next Step: Check for Outliers

Figure 2. Normality Screen for Trichloroethene Remediation Example 1, All Eight Data Points Used

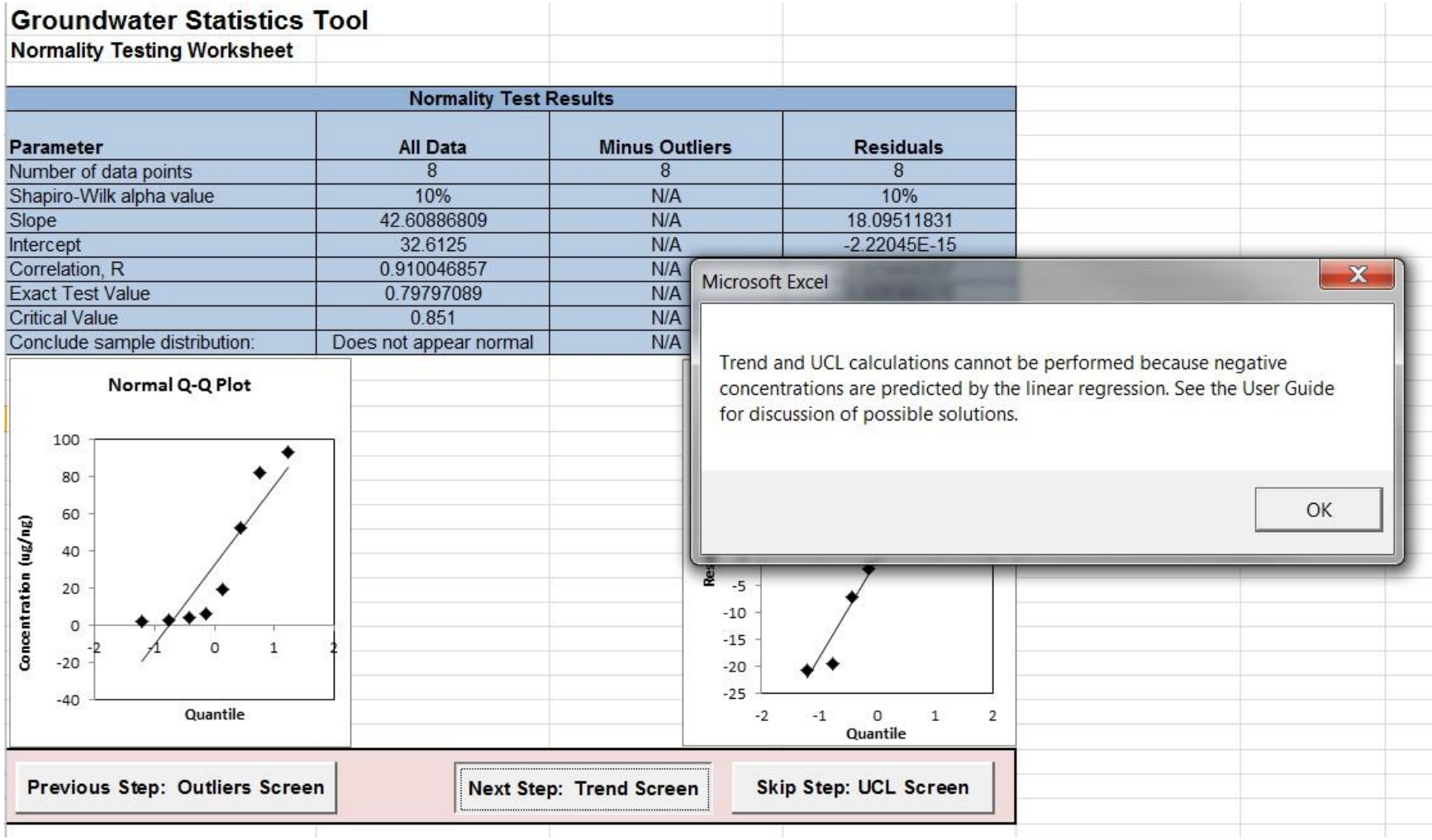


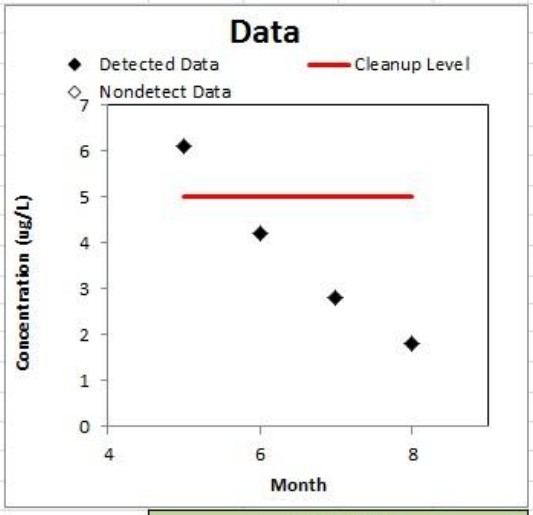
Figure 3. Data Input Screen for Trichloroethene Remediation Example 1, Final Four Data Points Used

Groundwater Statistics Tool

Data input worksheet

Site Name	Test
Operating Unit (OU)	Test
Type of Evaluation	Remediation
Date of Evaluation	6/11/2014
Person performing analysis	RT
Chemical of Concern	TCE
Well Name/Number	1
Date Units	Month
Concentration Units	ug/L
Confidence Level Desired	95%
Cleanup Level	5
Source of cleanup level (e.g. MCL or risk-based concentration)	MCL
Risk of False Outlier Rejection	1%
Random Seed (may be left blank)	62311.42188
Significant figures to use	3
Number of data points:	4
Number of detected results:	4
Number of nondetect results:	0
Detection frequency:	100%

Date (Month)	TCE Concentration (ug/L)	Data Qualifier	Detected? (Yes or No)
5	6.1		Yes
6	4.2		Yes
7	2.8		Yes
8	1.8		Yes



Axis Values			
Time		Concentration	
Min	Max	Min	Max
4	9	Auto	Auto

Reset Concentration Axis

Data Review		Recommendations
Are all necessary data fields entered, and in proper format?	Yes	None
Are at least 4 data points present for statistical analysis?	Yes	None
Are detection limits for nondetects ≤ maximum detected value?	Yes	None
Are all data within chart axis limits?	Yes	None

Pressing the "Check for Outliers" button to the right will open a worksheet that shows the results of a Dixons's test for outliers.

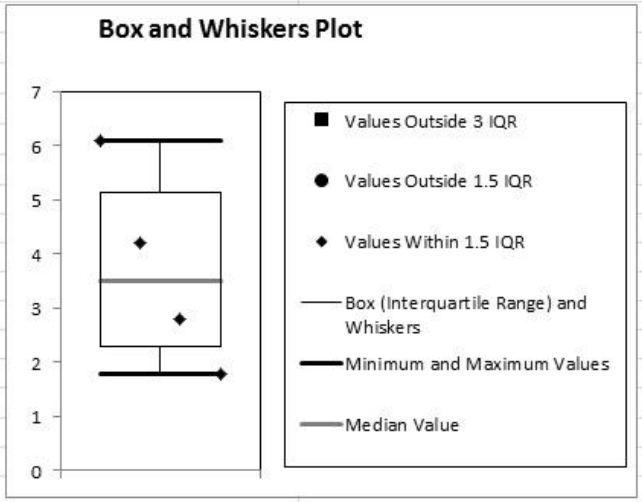
Next Step: Check for Outliers

Figure 4. Outlier Screen for Trichloroethene Remediation Example 1, Final Four Points Used

Groundwater Statistics Tool

Outlier testing worksheet

Dixon's Outlier Test Results		
Number of data points	4	
Risk of false rejection	1%	
Critical value	0.889	
Outlier type	**Low**	**High**
Test statistic	0.2326	0.4419
Potential Outlier?	No	No
Validity of Dixon'sTest	Valid	



Previous Step: Data Input Screen

Next Step: Normality Screen

Figure 5. Normality Screen for Trichloroethene Remediation Example 1, Final Four Points Used

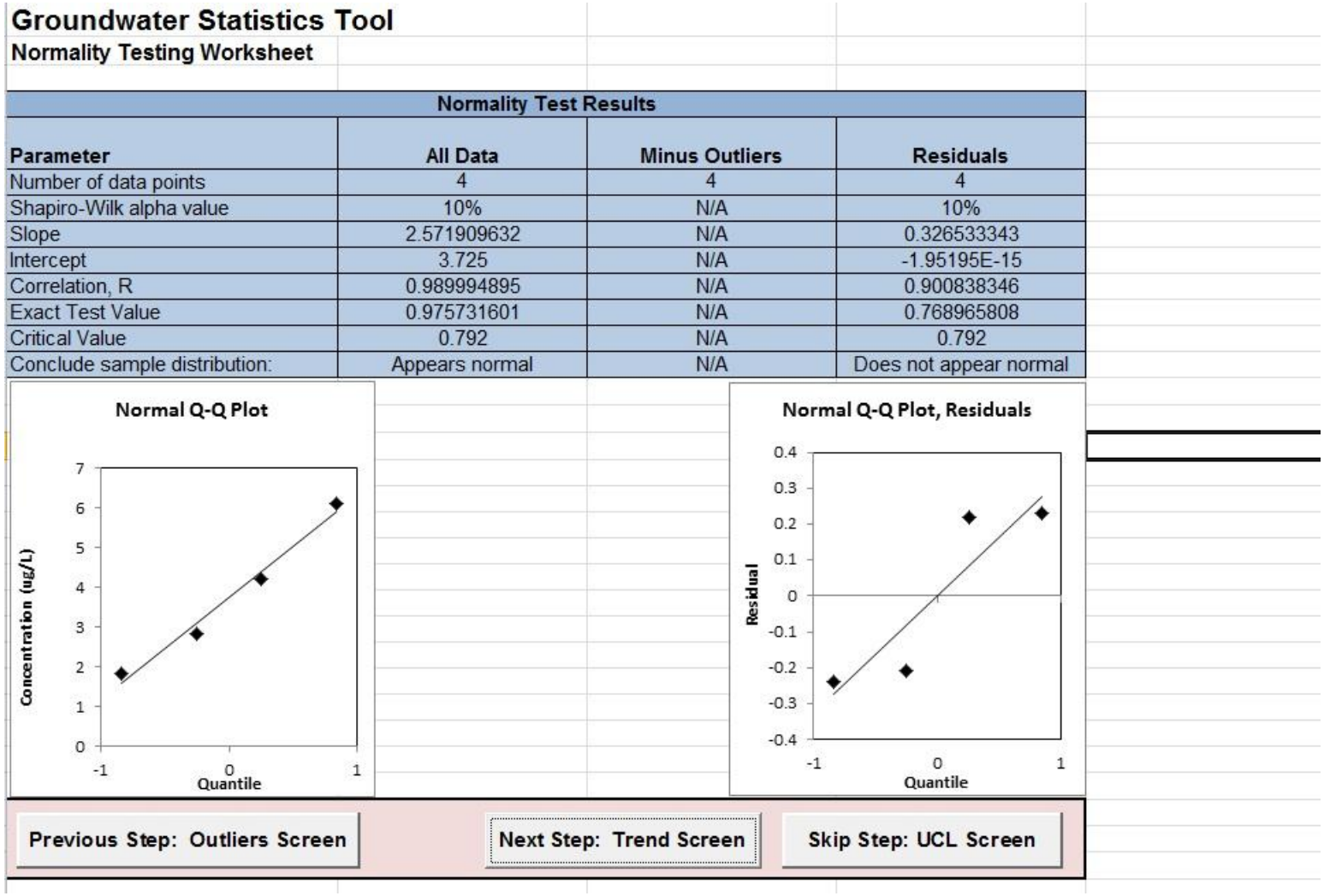


Figure 6. Trend Screen for Trichloroethene Remediation Example 1, Final Four Points Used

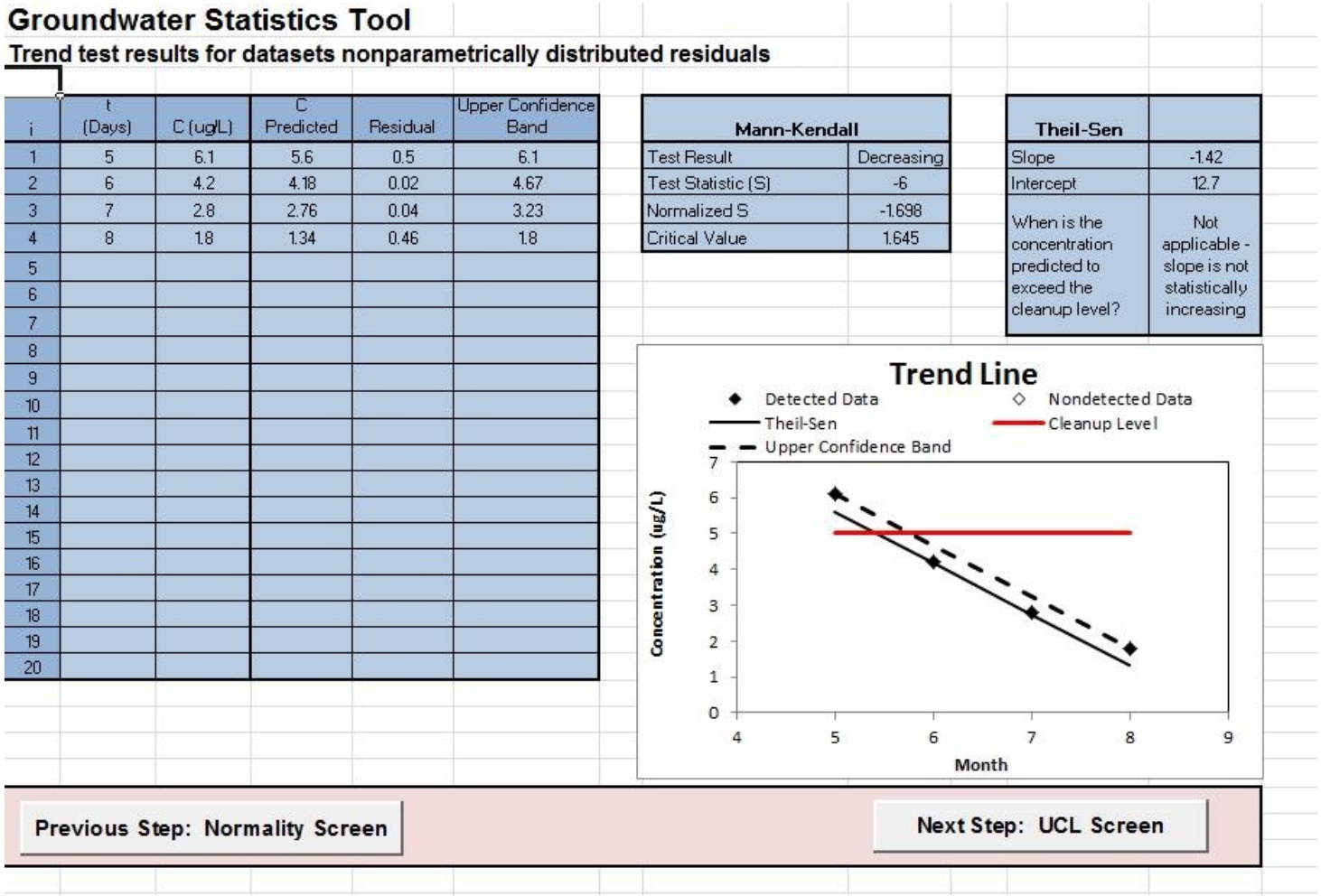


Figure 7. UCL Screen for Trichloroethene Remediation Example 1, Final Four Points Used

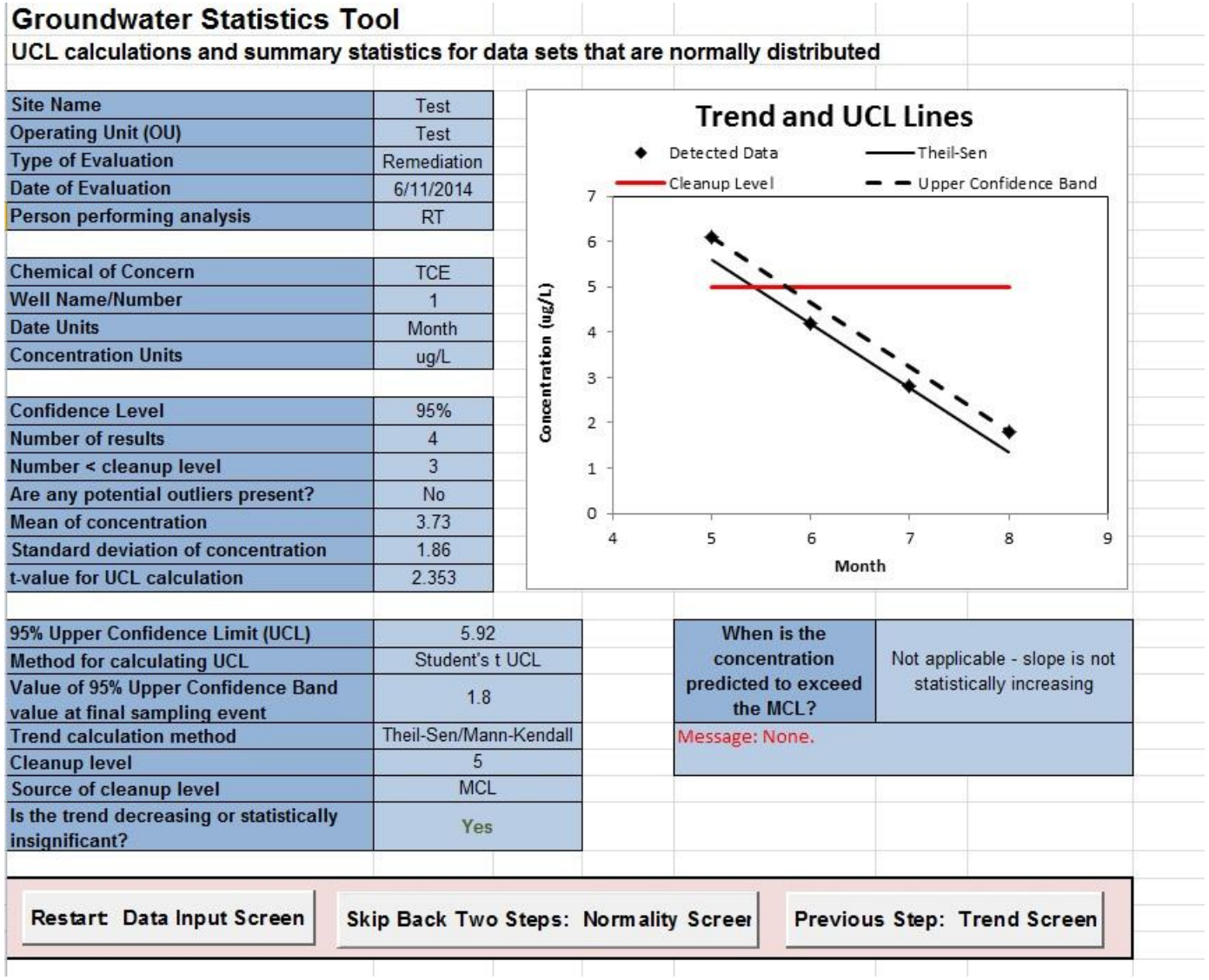


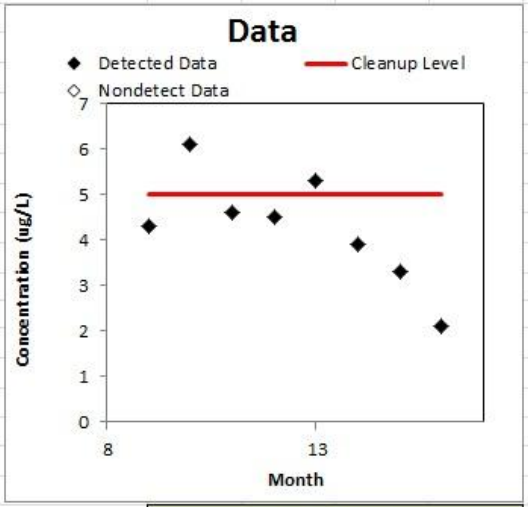
Figure 8. Data Input Screen for Trichloroethene Attainment Example 2, First Eight Data Points Used

Groundwater Statistics Tool

Data input worksheet

Site Name	Test
Operating Unit (OU)	Test
Type of Evaluation	Attainment
Date of Evaluation	6/11/2014
Person performing analysis	RT
Chemical of Concern	TCE
Well Name/Number	1
Date Units	Month
Concentration Units	ug/L
Confidence Level Desired	95%
Cleanup Level	5
Source of cleanup level (e.g. MCL or risk-based concentration)	MCL
Risk of False Outlier Rejection	1%
Random Seed (may be left blank)	62311.42188
Significant figures to use	3
Number of data points:	8
Number of detected results:	8
Number of nondetect results:	0
Detection frequency:	100%

Date (Month)	TCE Concentration (ug/L)	Data Qualifier	Detected? (Yes or No)
9	4.3		Yes
10	6.1		Yes
11	4.6		Yes
12	4.5		Yes
13	5.3		Yes
14	3.9		Yes
15	3.3		Yes
16	2.1		Yes



Axis Values			
Time		Concentration	
Min	Max	Min	Max
8	17	Auto	Auto

Reset Concentration Axis

Data Review		Recommendations
Are all necessary data fields entered, and in proper format?	Yes	None
Are at least 4 data points present for statistical analysis?	Yes	None
Are detection limits for nondetects ≤ maximum detected value?	Yes	None
Are all data within chart axis limits?	Yes	None

Pressing the "Check for Outliers" button to the right will open a worksheet that shows the results of a Dixons's test for outliers.

Next Step: Check for Outliers

Figure 9. UCL Screen for Trichloroethene Attainment Example 2, First Eight Data Points Used

Groundwater Statistics Tool

UCL calculations and summary statistics for data sets that are normally distributed

Site Name	Test
Operating Unit (OU)	Test
Type of Evaluation	Attainment
Date of Evaluation	6/11/2014
Person performing analysis	RT
Chemical of Concern	TCE
Well Name/Number	1
Date Units	Month
Concentration Units	ug/L
Confidence Level	95%
Number of results	8
Number < cleanup level	6
Are any potential outliers present?	No
Mean of concentration	4.26
Standard deviation of concentration	1.22
t-value for UCL calculation	1.895

95% Upper Confidence Limit (UCL)	5.08
Method for calculating UCL	Student's t UCL
Value of 95% Upper Confidence Band value at final sampling event	4.49
Trend calculation method	Ordinary Least Squares
Cleanup level	5
Source of cleanup level	MCL
Is the trend decreasing or statistically insignificant?	Yes

When is the concentration predicted to exceed the MCL?	Not applicable - slope is not statistically increasing
Message: None.	

Restart: Data Input Screen | Skip Back Two Steps: Normality Screer | Previous Step: Trend Screen

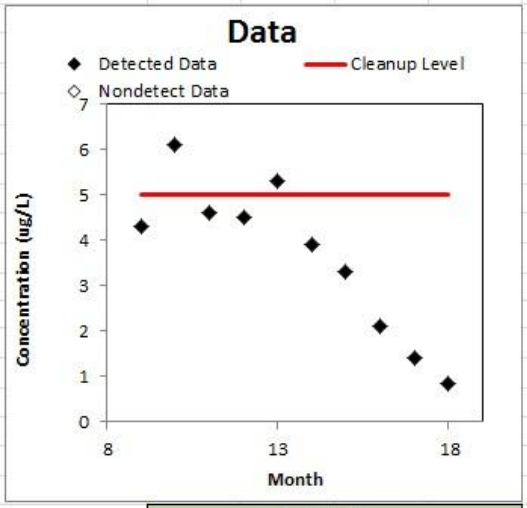
Figure 10. Data Input Screen for Trichloroethene Attainment Example 2, All Ten Data Points Used

Groundwater Statistics Tool

Data input worksheet

Site Name	Test
Operating Unit (OU)	Test
Type of Evaluation	Attainment
Date of Evaluation	6/11/2014
Person performing analysis	RT
Chemical of Concern	TCE
Well Name/Number	1
Date Units	Month
Concentration Units	ug/L
Confidence Level Desired	95%
Cleanup Level	5
Source of cleanup level (e.g. MCL or risk-based concentration)	MCL
Risk of False Outlier Rejection	1%
Random Seed (may be left blank)	62311.42188
Significant figures to use	3
Number of data points:	10
Number of detected results:	10
Number of nondetect results:	0
Detection frequency:	100%

Date (Month)	TCE Concentration (ug/L)	Data Qualifier	Detected? (Yes or No)
9	4.3		Yes
10	6.1		Yes
11	4.6		Yes
12	4.5		Yes
13	5.3		Yes
14	3.9		Yes
15	3.3		Yes
16	2.1		Yes
17	1.4		Yes
18	0.85		Yes



Axis Values			
Time		Concentration	
Min	Max	Min	Max
8	19	Auto	Auto

Reset Concentration Axis

Data Review		Recommendations
Are all necessary data fields entered, and in proper format?	Yes	None
Are at least 4 data points present for statistical analysis?	Yes	None
Are detection limits for nondetects ≤ maximum detected value?	Yes	None
Are all data within chart axis limits?	Yes	None

Pressing the "Check for Outliers" button to the right will open a worksheet that shows the results of a Dixons's test for outliers.

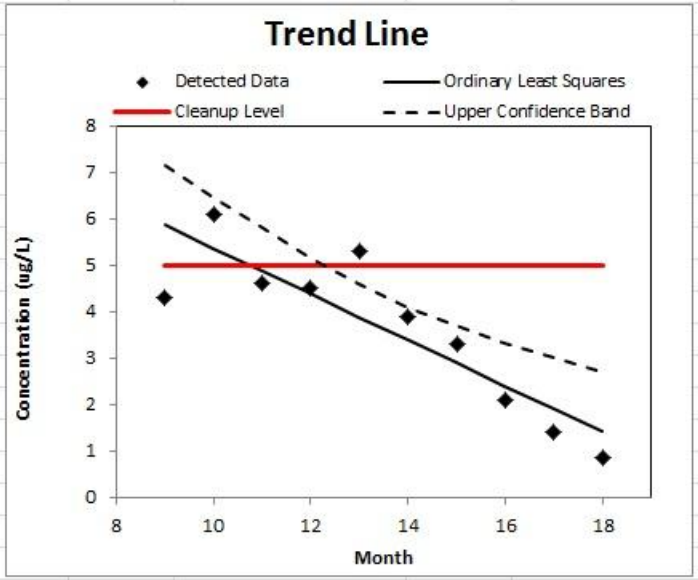
Next Step: Check for Outliers

Figure 11. UCL Screen for Trichloroethene Attainment Example 2, All Ten Data Points Used

Groundwater Statistics Tool

UCL calculations and summary statistics for data sets that are normally distributed

Site Name	Test
Operating Unit (OU)	Test
Type of Evaluation	Attainment
Date of Evaluation	6/11/2014
Person performing analysis	RT
Chemical of Concern	TCE
Well Name/Number	1
Date Units	Month
Concentration Units	ug/L
Confidence Level	95%
Number of results	10
Number < cleanup level	8
Are any potential outliers present?	No
Mean of concentration	3.64
Standard deviation of concentration	1.71
t-value for UCL calculation	1.833



95% Upper Confidence Limit (UCL)	4.63
Method for calculating UCL	Student's t UCL
Value of 95% Upper Confidence Band value at final sampling event	2.7
Trend calculation method	Ordinary Least Squares
Cleanup level	5
Source of cleanup level	MCL
Is the trend decreasing or statistically insignificant?	Yes

When is the concentration predicted to exceed the MCL?	Not applicable - slope is not statistically increasing
Message: None.	

Restart: Data Input Screen | Skip Back Two Steps: Normality Screer | Previous Step: Trend Screen

Figure 12. Data Input Screen for Vinyl Chloride Remediation Example 3

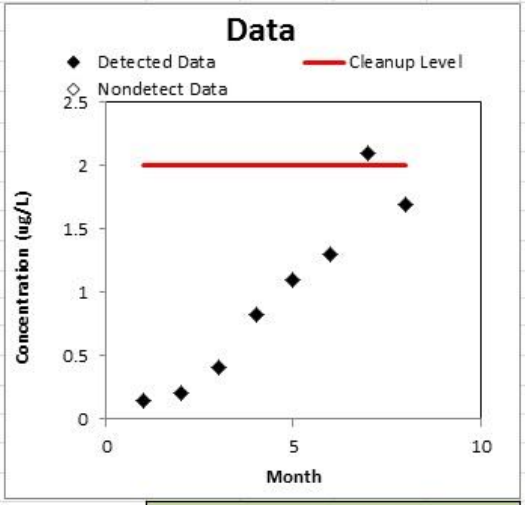
Groundwater Statistics Tool

Data input worksheet

Site Name	Test
Operating Unit (OU)	Test
Type of Evaluation	Remediation
Date of Evaluation	6/11/2014
Person performing analysis	RT
Chemical of Concern	VC
Well Name/Number	1
Date Units	Month
Concentration Units	ug/L
Confidence Level Desired	95%
Cleanup Level	2
Source of cleanup level (e.g. MCL or risk-based concentration)	MCL
Risk of False Outlier Rejection	1%
Random Seed (may be left blank)	62311.42188
Significant figures to use	3

Number of data points:	8
Number of detected results:	8
Number of nondetect results:	0
Detection frequency:	100%

Date (Month)	VC Concentration (ug/L)	Data Qualifier	Detected? (Yes or No)
1	0.15		Yes
2	0.21		Yes
3	0.41		Yes
4	0.82		Yes
5	1.1		Yes
6	1.3		Yes
7	2.1		Yes
8	1.7		Yes



Axis Values			
Time		Concentration	
Min	Max	Min	Max
Auto	Auto	Auto	Auto

Reset Concentration Axis

Data Review		Recommendations
Are all necessary data fields entered, and in proper format?	Yes	None
Are at least 4 data points present for statistical analysis?	Yes	None
Are detection limits for nondetects ≤ maximum detected value?	Yes	None
Are all data within chart axis limits?	Yes	None

Pressing the "Check for Outliers" button to the right will open a worksheet that shows the results of a Dixons's test for outliers.

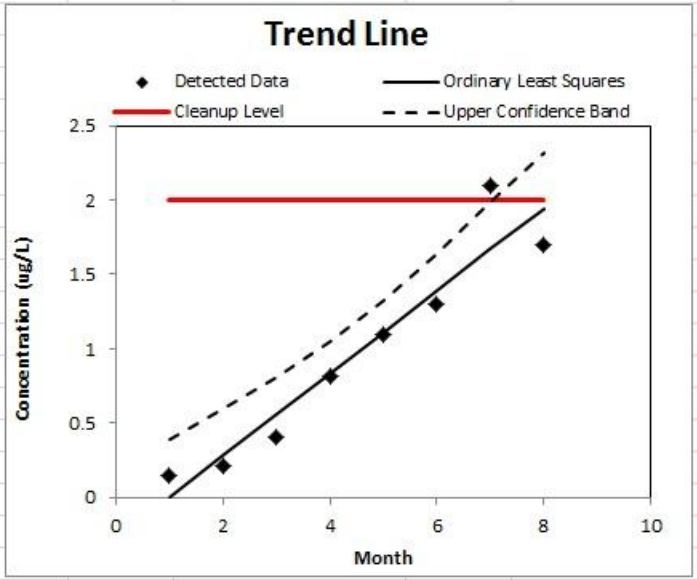
Next Step: Check for Outliers

Figure 13. UCL Screen for Vinyl Chloride Remediation Example 3

Groundwater Statistics Tool

UCL calculations and summary statistics for data sets that are normally distributed

Site Name	Test
Operating Unit (OU)	Test
Type of Evaluation	Remediation
Date of Evaluation	6/11/2014
Person performing analysis	RT
Chemical of Concern	VC
Well Name/Number	1
Date Units	Month
Concentration Units	ug/L
Confidence Level	95%
Number of results	8
Number < cleanup level	7
Are any potential outliers present?	No
Mean of concentration	0.974
Standard deviation of concentration	0.709
t-value for UCL calculation	1.895



95% Upper Confidence Limit (UCL)	1.45
Method for calculating UCL	Student's t UCL
Value of 95% Upper Confidence Band value at final sampling event	2.32
Trend calculation method	Ordinary Least Squares
Cleanup level	2
Source of cleanup level	MCL
Is the trend decreasing or statistically insignificant?	No

When is the concentration predicted to exceed the MCL?	8.21
Message: None.	

Restart Data Input Screen | Skip Back Two Steps: Normality Screer | Previous Step: Trend Screen

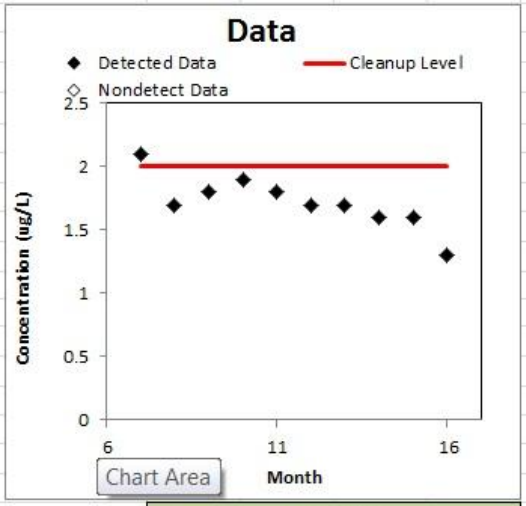
Figure 14. Data Input Screen for Vinyl Chloride Attainment Example 4

Groundwater Statistics Tool

Data input worksheet

Site Name	Test
Operating Unit (OU)	Test
Type of Evaluation	Attainment
Date of Evaluation	6/11/2014
Person performing analysis	RT
Chemical of Concern	VC
Well Name/Number	1
Date Units	Month
Concentration Units	ug/L
Confidence Level Desired	95%
Cleanup Level	2
Source of cleanup level (e.g. MCL or risk-based concentration)	MCL
Risk of False Outlier Rejection	1%
Random Seed (may be left blank)	62311.42188
Significant figures to use	3
Number of data points:	10
Number of detected results:	10
Number of nondetect results:	0
Detection frequency:	100%

Date (Month)	VC Concentration (ug/L)	Data Qualifier	Detected? (Yes or No)
7	2.1		Yes
8	1.7		Yes
9	1.8		Yes
10	1.9		Yes
11	1.8		Yes
12	1.7		Yes
13	1.7		Yes
14	1.6		Yes
15	1.6		Yes
16	1.3		Yes



Axis Values			
Time		Concentration	
Min	Max	Min	Max
6	17	Auto	Auto

Reset Concentration Axis

Data Review		Recommendations
Are all necessary data fields entered, and in proper format?	Yes	None
Are at least 4 data points present for statistical analysis?	Yes	None
Are detection limits for nondetects ≤ maximum detected value?	Yes	None
Are all data within chart axis limits?	Yes	None

Pressing the "Check for Outliers" button to the right will open a worksheet that shows the results of a Dixons's test for outliers.

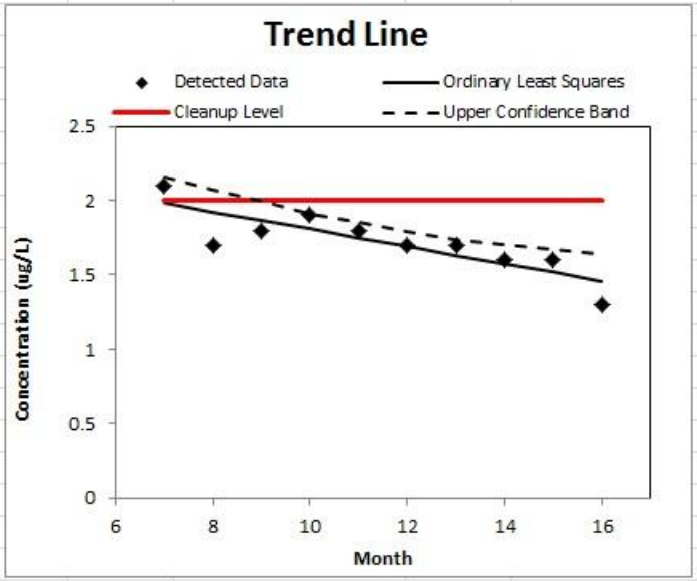
Next Step: Check for Outliers

Figure 15. UCL Screen for Vinyl Chloride Attainment Example 4

Groundwater Statistics Tool

UCL calculations and summary statistics for data sets that are normally distributed

Site Name	Test
Operating Unit (OU)	Test
Type of Evaluation	Attainment
Date of Evaluation	6/11/2014
Person performing analysis	RT
Chemical of Concern	VC
Well Name/Number	1
Date Units	Month
Concentration Units	ug/L
Confidence Level	95%
Number of results	10
Number < cleanup level	9
Are any potential outliers present?	No
Mean of concentration	1.72
Standard deviation of concentration	0.21
t-value for UCL calculation	1.833



95% Upper Confidence Limit (UCL)	1.84
Method for calculating UCL	Student's t UCL
Value of 95% Upper Confidence Band value at final sampling event	1.64
Trend calculation method	Ordinary Least Squares
Cleanup level	2
Source of cleanup level	MCL
Is the trend decreasing or statistically insignificant?	Yes

When is the concentration predicted to exceed the MCL?	Not applicable - slope is not statistically increasing
Message: None.	

Restart Data Input Screen | Skip Back Two Steps: Normality Screen | Previous Step: Trend Screen