USER GUIDE:

LITERATURE REVIEW AND SOFTWARE DEVELOPMENT FOR GROUNDWATER AND SURFACE WATER QUALITY TREND ANALYSES

Prepared for:
BGC Engineering Inc.

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Abstract

In this study project, a software program was developed which aims to serve as a tool for scientists in assessing trends in groundwater and surface water quality parameters. Particular challenges face decision-makers when assessing environmental datasets for trends. While a large number of statistical trend analysis methods for environmental data are available, comprehensive guidance and software for best practices in computing trend analyses are not readily available. Further, data are rarely well-behaved in fitting assumed distribution models, may be collected at sporadic or discontinuous intervals, often contain non-detects and can consist of underlying seasonal, autocorrelative as well as stochastic patterns (Ofungwu, 2014). This study project was carried out with the goal of helping to address this documentation and software gap by assembling relevant documented literature and applying best practices in a prepared software package. The software was then applied to a case study project, from surface water data collected from the Adige catchment in northern Italy.

Documented methods for trend analyses on environmental data were first researched. The methods of maximum likelihood estimation (MLE) linear regression (using normal, lognormal and gamma distributions) as well as variations of the Mann-Kendall trend test (implemented for seasonal data as well as corrected for data which is autocorrelated) in combination with a determination of Theil-Sen and Akritas-Theil-Sen slopes were then chosen for implementation in a developed software program, as these are common methods which are capable of processing non-detect values common in environmental datasets.

The resulting software is able to read and process data sets containing non-detect values and “greater-than” values, as flagged in a dataset by the symbols “<” and “>”. Linear regression, Mann-Kendall analyses as well as a determination of Akritas-Theil-Sen slope is then carried out without substituting censored values and without resulting in the loss of data.

The case study carried out on Italy’s Adige catchment highlighted the value of applying a variety of approaches in trend analysis on a dataset, and the developed software presents a tool for implementing varied trend analysis approaches.

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1 Introduction

Increasingly, parties responsible for carrying out environmental monitoring as well as environmental regulators alike are becoming interested in changes in environmental quality parameters over time, rather than simply static parameter values in relation to a prescribed guideline. These trend analyses can be carried out in a number of different ways (regression, Mann-Kendall, varying spatial and temporal averaging approaches, etc.). In addition, environmental datasets are particularly rarely well-behaved, with non-detects, outliers, skewness and/or seasonal patterns often present (Ofungwu, 2014). Documentation and software for best practices for conducting environmental trend analyses are not, however, readily available. This study project was thus carried out with the goal of helping to address this documentation and software gap by assembling relevant documented literature and applying best practices in a prepared software package. The software was then applied to a case study project, from surface water data collected from the Adige catchment in Northern Italy.

While there is a range of environmental data analysis software applications available, many tend to be designed for large-scale and long-term projects and involve high initial costs (Jones et al., 2014). Other free or low-cost programs are often inflexible. In addition, methods implemented in available software often do not reflect modern best trend analysis practices, as trend analysis capabilities are often included as an afterthought in software packages which focus rather on data management and/or on determining summary statistics. It was thus aimed that the software researched and developed as part of this study project could provide a rigorous and defensible tool for trend analyses on groundwater and surface water datasets.

This study project was carried out in partial fulfilment of the requirements of the Environmental Engineering MSc. Programme of the Technical University of Munich (TUM, Germany). The project consisted of a literature and software review phase (refer to Appendix A), a software development phase and a case study implementation phase to test the developed software on a surface water dataset from the Adige catchment, in northern Italy (Appendices B & C).

2 Data Input Requirements

The software developed in the course of this study project has been set up to read databases which are stored as Excel files (.xls). Data entries should be stored as rows, where each column represents a data field. Though the user is free to choose the exact naming convention of the columns, the fields included should generally be, at a minimum:

- Sampling date
- Well or station ID
- Contaminant of concern concentration value (where non-detect values or greater-than values are recognized by the symbols “<” and “>” next to a concentration value, where applicable)

Other considerations are:

- Group ID, when analyses are to be performed on groups of stations, rather than individual stations.

In parallel with the analysis data requirements, extreme importance should be stressed in data collection and database setup on consistency in nomenclature and formatting in order for analyses to be carried out smoothly. Stations ID’s should be referred to exactly consistently (Station-1 or station 01 versus Station_01, for example) and date formats must be consistent.

2.1 Minimum Data Requirements

Linear Regression: USEPA (2013) has recommended that at least 10 observations should be available for hypotheses testing approaches. USEPA has further published in their *Unified Guidance for Statistical Analysis of Groundwater Monitoring at RCRA Facilities* (2009) that for linear regressions and for Mann-Kendall analyses, at least 8-10 observations should be available.

Mann-Kendall type trend tests can be carried out on data sets with as few as three observations. However, significant (at significance of 0.1) trends can only be deduced when at least four data points are avaiable.

For **seasonal Mann-Kendall** analyses, Helsel and Hirsch (2002) have stated that when the product of the number of seasons and the number of years of observations is at least 25, the distribution of the S statistic can be well approximated by a normal distribution. Guidance regarding seasonal Mann-Kendall tests on data containing less than 25 sampling events and which may contain data ties is not readily available.

Mann-Kendall, Correction for Autocorrelated data: since the correction is applied to the variance value of the S statistic (refer to Appendix A), the correction is only applicable when the S statistic approximately follows a normal distribution ($n>10$, or $n\geq25$ for a seasonal Mann-Kendall test)

3 Program Guide

3.1 Installation

To run, run the file “MyAppInstaller_web” first (this only needs to be done once per pc) and then download and run the “EnvTrend_V1” file to launch the program. The program may be slow to start-up and to get from the first window to the second upon the first launch (less than ~20 seconds, but this can feel like a long time). Once past the first interface window, the user can then quickly switch between analyses, but is advised to close one result window before opening a new one. If program fails to launch, try running as an administrator (right click -> “Run as administrator”).

3.2 Initial Interface

In the initial interface (Figure 2.1), the user is prompted to select a file in which the data is contained. The software has been set up to read from .xls-based databases (Microsoft Excel). Files containing multiple spreadsheets are supported, as the user is then prompted to specify the sheet which contains the data to be analysed.

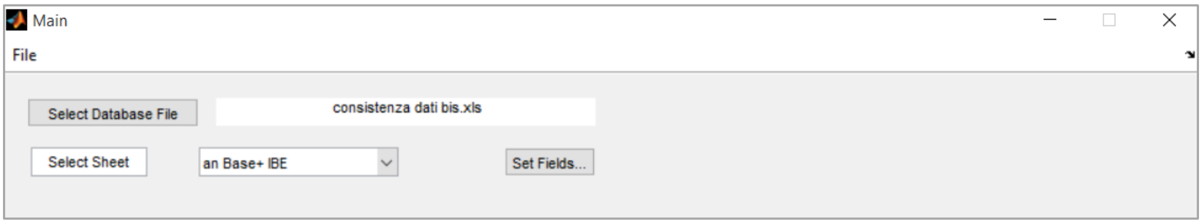

Figure 2.1 Initial Interface.

3.3 Defining Fields

Once data have been loaded from the specified spreadsheet (may take a few seconds for large databases), the user is then taken to the next interface (Figure 2.2) in order to define the fields of the database which are required for the trend analyses. A sample of the data is displayed in the interface in order to assist with defining the fields. Here, the user specifies the number of header rows to be read and defines the required fields “Station ID’s”, “Sampling Date”, “Date Format” as well as the analysis parameter. Gaps or blank entries in a data set are supported. Text characters which are stored in the analysis parameter field (with the exception of the symbols ‘<’ or ‘>’) will be ignored.

Further options (not required) include:

- Maximum length of sampling event: In the case that individual sampling events span more than one day (for example, a bi-annual sampling program which runs over the course of a week, twice per year), the user has the option here to enter a threshold for which sampling events should be grouped together. This is only important in the case where groups of wells are to be analysed together, but some sampling events may have occurred a day or two apart. For example, for a biannual sampling program where samples from a site could be collected over a period of seven days, twice a year, the value here would be seven in order to ensure that samples collected only seven days apart are considered as ties in the time domain

- Station Grouping: Here, the user can set groups of stations, for which analyses will also be carried out. These can be defined in a separate field within the database, or a maximum of four groups can be defined manually within the interface.

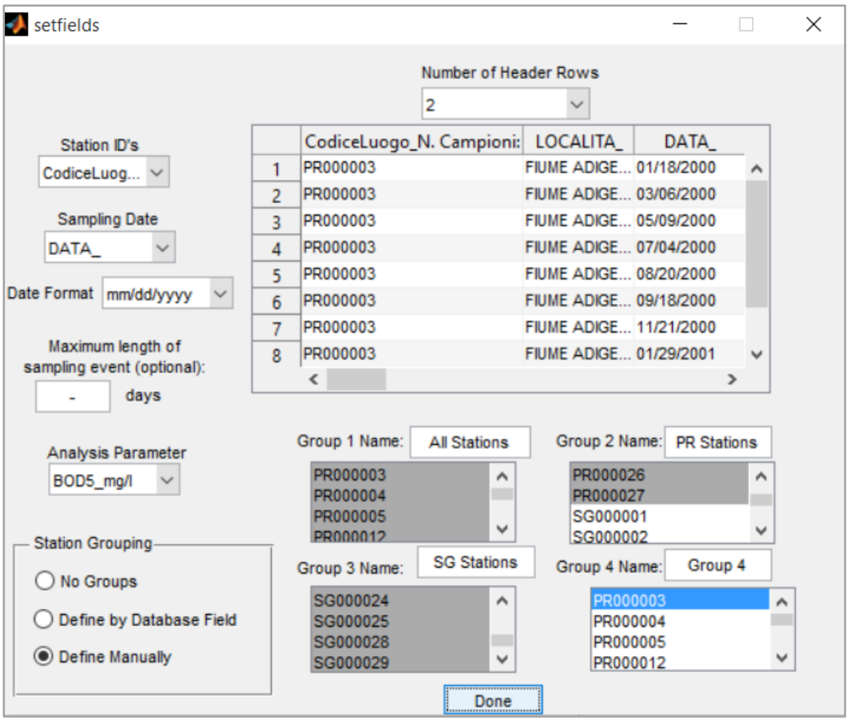

Figure 2.2 Interface for defining database fields.

3.4 Analysis Setup

In the next interface (Figure 2.3), the user is prompted to select whether an MLE linear regression or a Mann-Kendall test is to be carried out. In the case of a Mann-Kendall test, the user can then define whether the test should be carried out as a normal test or as a seasonal Mann-Kendall test. When a seasonal Mann-Kendall test is selected, the seasons must also be defined. Season options include: monthly, per season (Winter, Spring, Summer and Fall), two seasons per year (Winter/Spring and Summer/Fall) or up to twelve user-defined seasons. In the analysis setup interface, the user must also specify on which stations, or station groups, the analyses are to be carried out and can set the desired significance level for the trend tests (default is 0.05).

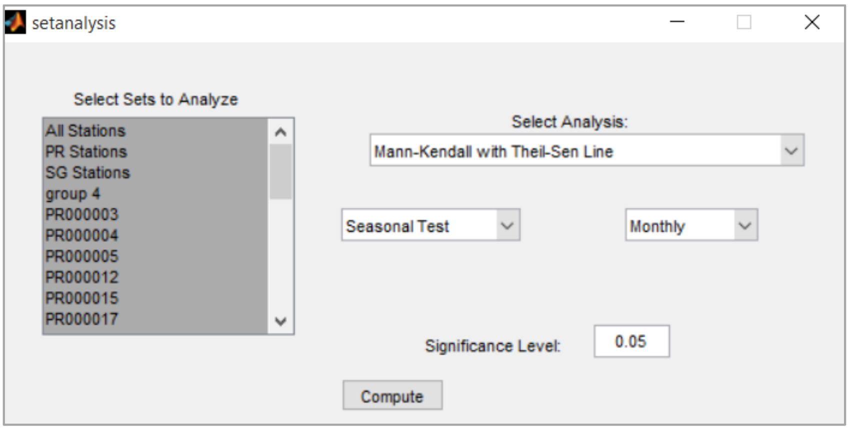

Figure 2.3 Analysis setup interface.

3.5 Output Interface: Linear Regression

When the user has selected a linear regression trend analysis and proceeded with the analysis, the linear regression output will display a graph with three lines, as in Figure 2.4. The three lines correspond to linear regressions on the dataset assuming a (1) normal, (2) lognormal and (3) gamma distribution of the data residuals. In the plot, detected data values, non-detect values (plotted at their detection limit) as well as the fitted MLE linear model are displayed.

The interface further displays the p-value of the corresponding test and, if the p-value is lower than the user-specified significance level, the slope of the trend as estimated by the model. Note that for the normal and gamma distributions, the units of the regression slope value are in (input units)/year, while the units for the lognormal distribution are in % change/year.

In order to view how well the residuals fit each of the specified distributions, the user can click on the "View Residual Probability Plot" control button and a new window will appear with a probability plot of the residuals (Figure 2.5). With the probability plots, the user can assess which of the distributions represents a better fit for the data model.

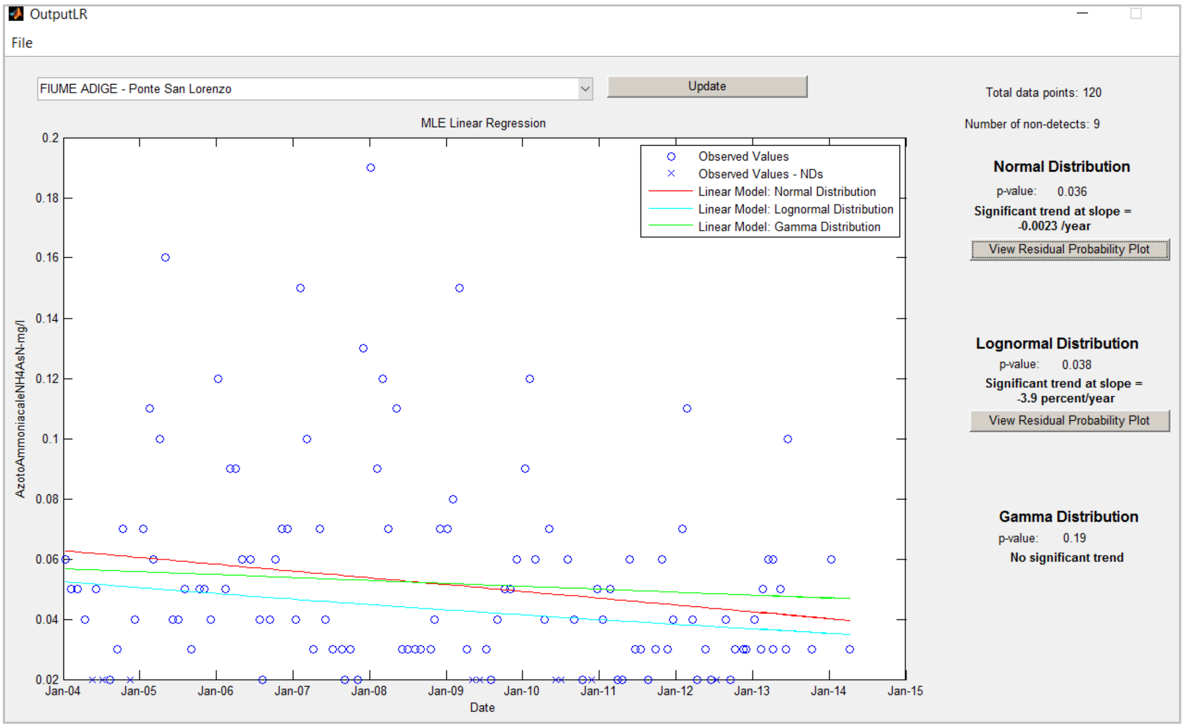

Figure 2.4 Linear regression output interface.

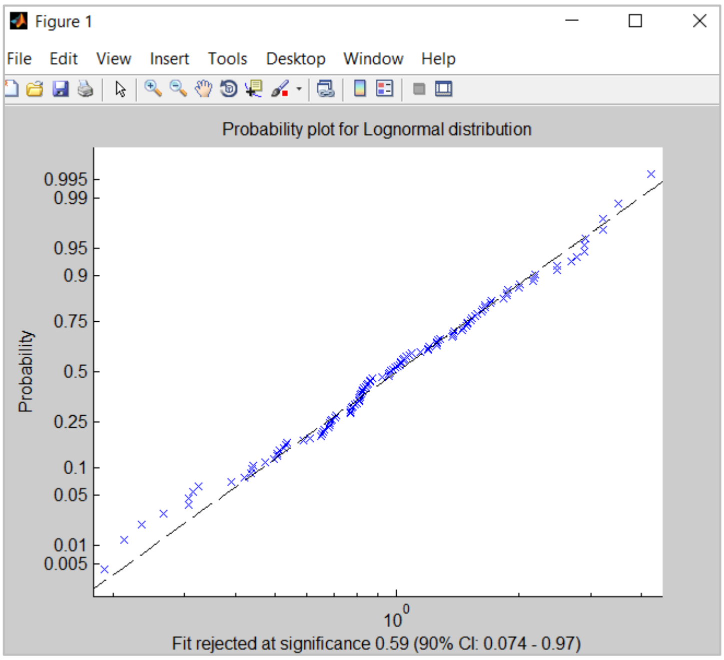

Figure 2.5 Probability plot for specified distribution (in this case: lognormal).

In the probability plot output, the user is provided, at the bottom of the graph, with a range of p-values resulting from a Chi-squared test which has tested the goodness of fit of the residuals to the respective model. The Chi-squared test has been carried out using a default of 10 bins, and a minimum count of 3 expected observations per bin (neighbouring bins are pooled when this is not met). For very small data sets (n≤15), the Chi-squared test is carried out using 3 bins.

The Chi-square test evaluates the null-hypothesis that the residuals follow the specified trend and rejects this hypothesis only at the specified significance (i.e. for a typical desired significance of 0.05, it would be concluded that the given distribution does **not** fit the residuals when the outputted range is below 0.05. If the range is above 0.05, such as in Figure 6.5, it is not rejected that the given distribution fits the data residuals.)

A range is outputted in this interface as a result of the uncertainty associated with the non-detect observations. The Chi-square test is in fact carried out 1000 times, each time with random values between 0 and the detection limit (distributed according to the assumed distribution) replacing each of the non-detect values. The outputted value represents the median significance of the goodness of fit test from all 1000 trials. A range representing the mid-90% interval of these 1000 p-values is also outputted.

3.6 Output Interface: Mann-Kendall Test

In the output interface for the Mann-Kendall trend test, a single graph is displayed which contains the observed values as well as the computed Akritas-Theil-Sen slope for the dataset. To the right of the graph, both the computed Akritas-Theil-Sen slope and a range of possible Theil-Sen slopes is displayed.

In computing the Theil-Sen slope, non-detects have been replaced by random values (uniform distribution) between 0 and the respective detection limits and the resulting Theil-Sen line has been computed 1000 times. When non-detects are present, a range is output representing the mid-90% interval of these 1000 trials.

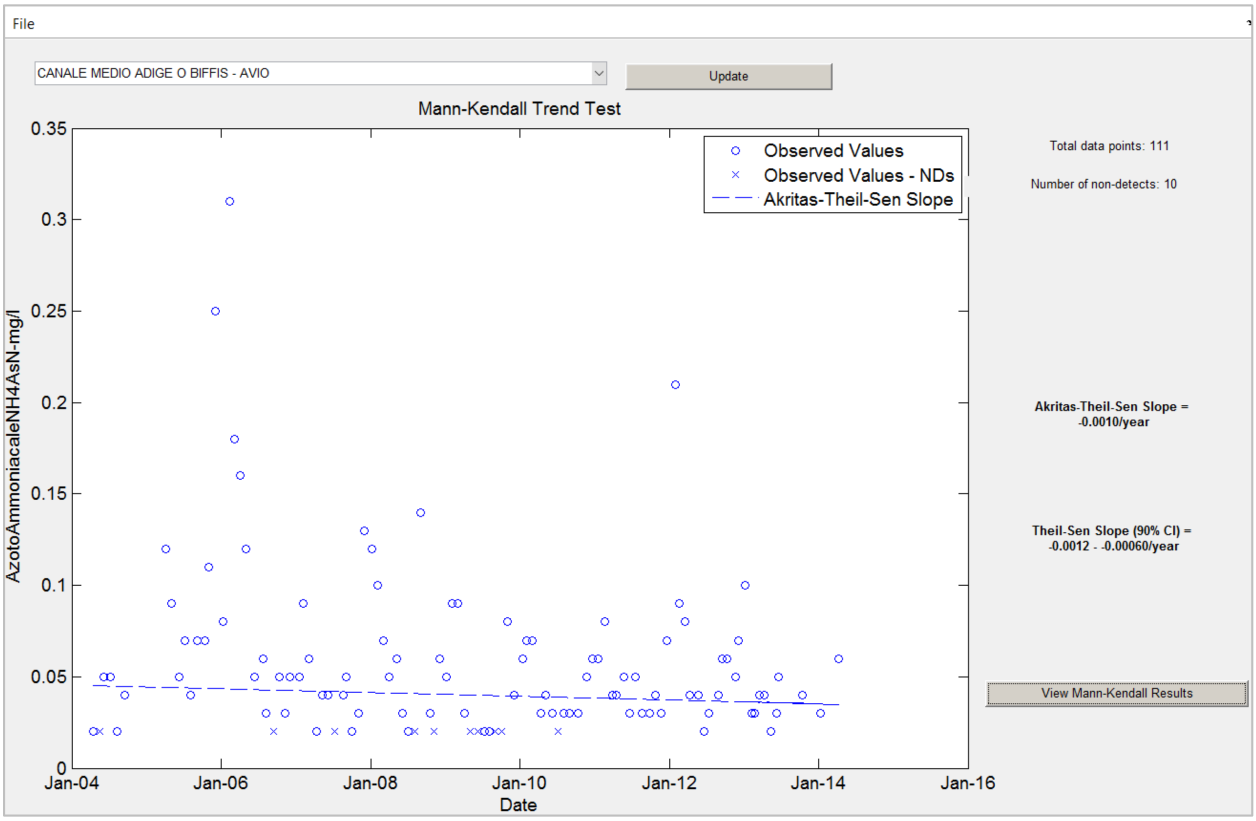

Figure 2.6 Mann-Kendall trend test output interface.

Through the control button labelled "View Mann-Kendall Results", the user can view the results of the Mann-Kendall test as well as a plot of the lag-values versus the respective autocorrelations on the data ranks. The autocorrelation plot should help the user to assess whether the corrected or the uncorrected test results are most appropriate for the dataset. This displayed autocorrelation function is the function which has been used to compute the corrected Mann-Kendall trend test. When autocorrelation in the dataset is plausible and evidenced by the autocorrelation plot, the corrected Mann-Kendall result is more appropriate for the data set.

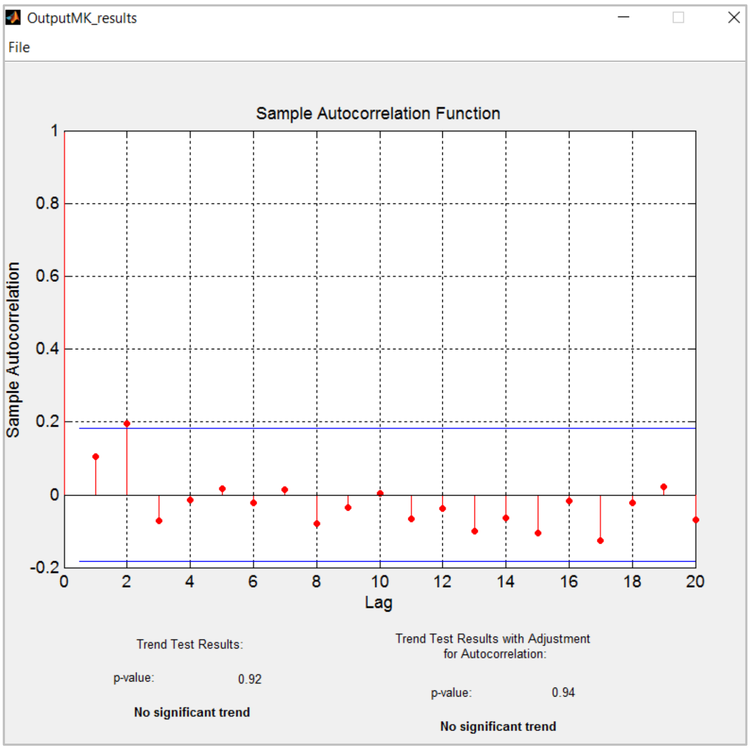

Figure 2.7 Mann-Kendall results interface as well as autocorrelation function of data ranks used to compute Mann-Kendall test corrected for autocorrelation.

3.7 Output Interface: Seasonal Mann-Kendall Test

The interface for the output of the seasonal Mann-Kendall test (Figure 2.8) is very similar to the interface for the Mann-Kendall test, except the results refer to a seasonal trend analysis and Theil-Sen/Akritas-Theil-Sen slope estimates have been computed for each of the respective seasons. In the autocorrelation function display (Figure 2.9), a separate plot is shown for each season, since the corrected variance values in the seasonal test are summed for each of the seasons. The autocorrelation functions displayed thus represent the functions which have been used to compute the corrected variance for each of the seasons.

In computing the Theil-Sen slope for each season, non-detects have been replaced by random values (uniform distribution) between 0 and the respective detection limits and the resulting Theil-Sen line has been computed 1000 times. When non-detects are present, a range is output representing the mid-90% interval of these 1000 trials for the Theil-Sen slope. Data pairs in a set which have been collected in the same season and year are excluded in computing the Theil-Sen and Akritas-Theil-Sen slopes and are considered ties in computing the Mann-Kendall test.

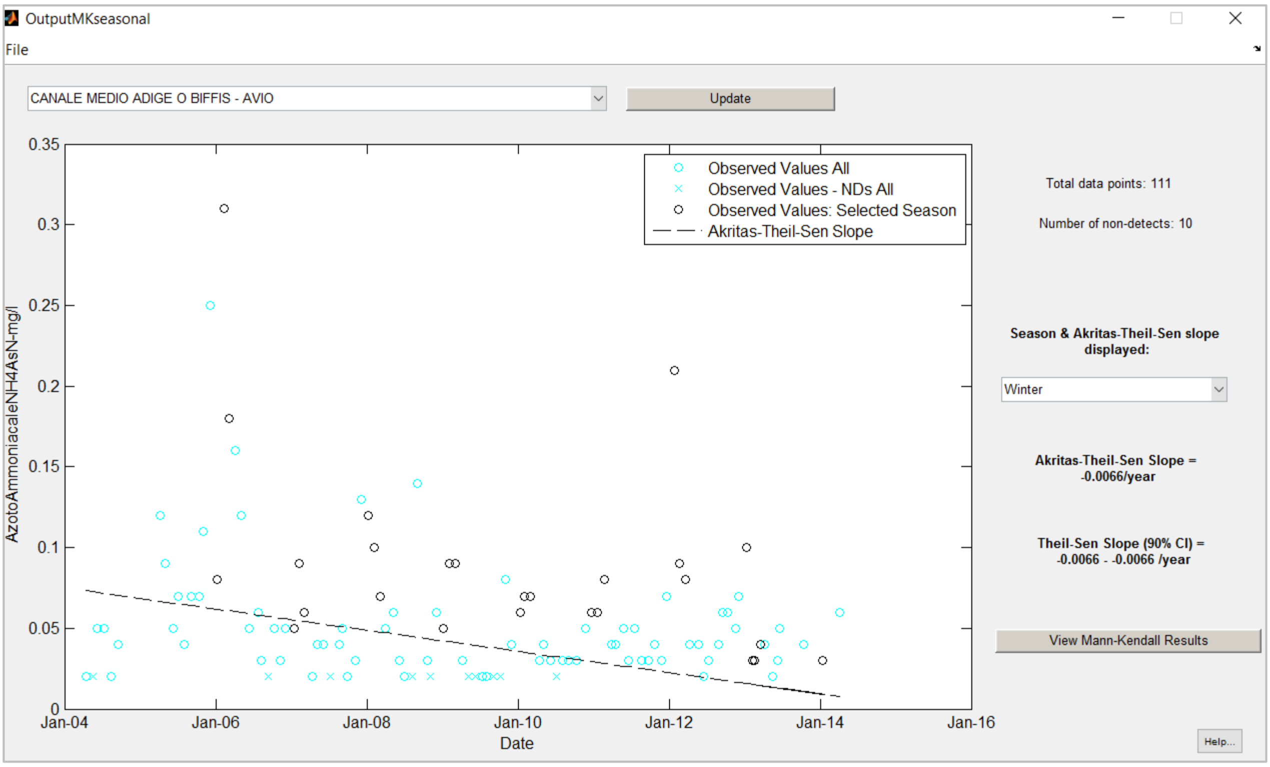

Figure 2.8 Seasonal Mann-Kendall trend test output interface.

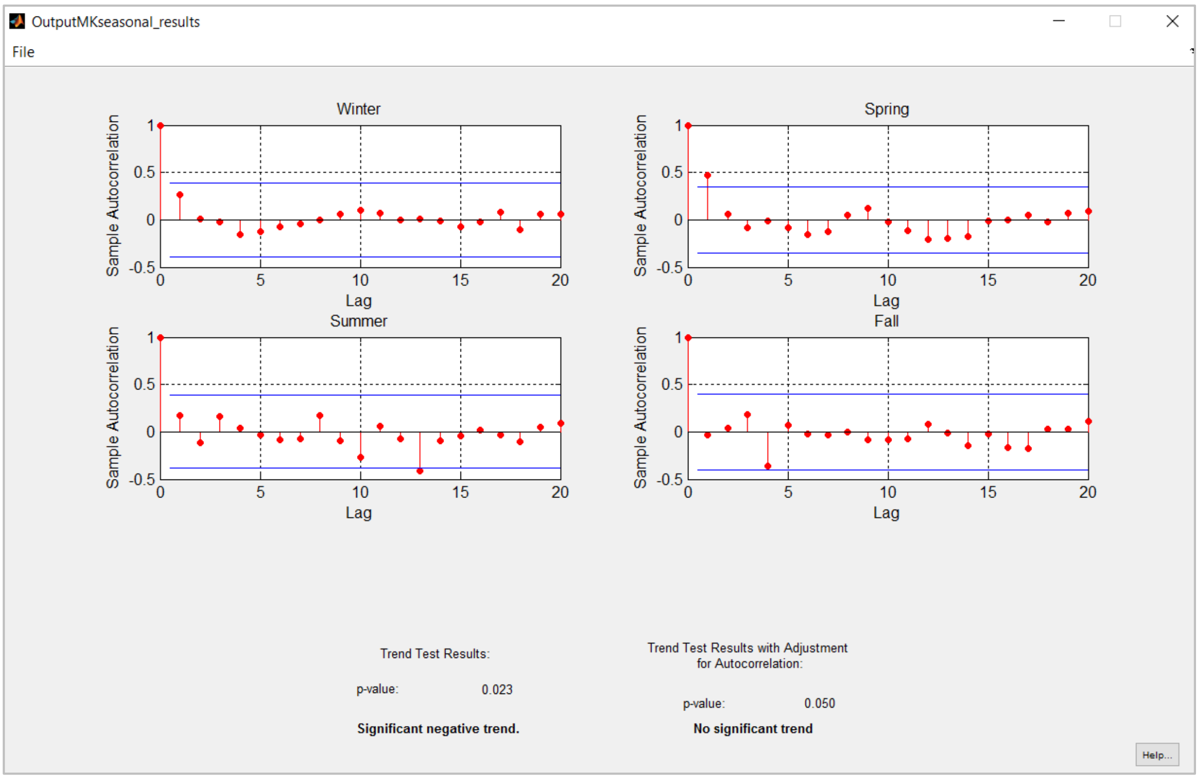

Figure 2.9 Autocorrelation function of data ranks used to compute corrected seasonal Mann-Kendall test.

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Prof. Dr. Markus Disse

APPENDIX A - TECHNICAL BACKGROUND:

LITERATURE REVIEW AND SOFTWARE DEVELOPMENT FOR GROUNDWATER AND SURFACE WATER QUALITY TREND ANALYSES

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Nomenclature

Abbreviations

KM	Kaplan-Meier
MLE	Maximum Likelihood Estimation
ROS	Regression on Order Statistics
TUM	Technical University of Munich
USEPA	United States Environmental Protection Agency

Mathematical Notations

b_0, b_1	Parameters (intercept, slope) of linear regression
cov	Coefficient of variation
f, F	Normal probability density function and cumulative distribution function
G^2	Log-likelihood test statistic
k	Shape parameter of gamma distribution
L	Log-likelihood
m	Number of seasons in seasonal Mann-Kendall test
n, n_d, n_{nd}, n_{md}	Number of observations (general, uncensored, left-censored and right-censored)
N_c, N_D	Number of concordant and discordant pairs in a dataset, respectively
$\frac{n}{n_S^*}$	Correction factor due to autocorrelation
p, P	Gamma probability density function and cumulative distribution function
Q	Theil-Sen slope

$R_t^{(X)}$, $R_t^{(Y)}$	Ranks of variables *x* and *y* at time *t*, respectively
S	Mann-Kendall test statistic
$S(d^2)$	Sum of squared differences
t	Time
t_i, ui	Extent of data ties in the time domain and concentration domain, respectively
T_i	Pair-wise slope *i*
$Var^*[S]$	Variance of S corrected for autocorrelation
y	Analysis parameter, typically concentration
Z	Normalized Z statistic
$\rho_s(i)$	Autocorrelation function of observation ranks
θ	Scale parameter of gamma distribution
σ	Standard deviation
π	Probability of concentration being above greater than or equal to specified value

1 Introduction

The focus of this Study Project was to develop a rigorous and defensible tool for trend analyses. In order to accomplish this, a litterature review was first carried out in order to identify best practices in trend analysis. From this, methods were selected which were to be implemented in the developped software application. Existing software were also researched and reviewed in the literature review phase in order to provide a context for the project. Finally, the software with the selected trend analysis capabilities was developped in Matlab R2013b and then compiled for distribution as a .exe file. The resulting software was then tested on the case study dataset, surface water data from the Adige catchment.

2 Literature Review

2.1 Censored Data: Handling Non-Detects

Particular complexity in carrying out trend analyses on water quality datasets is attributed to the frequent presence of non-detect values in datasets. When the exact value of a data point is not known, but rather, information is known regarding some range within which the data point falls (i.e. less than the detection limit or, in some cases, greater than the reporting limit), the data is referred to as censored. More specifically, data points which are defined as being less than a given detection limit are referred to as left-censored. Right-censored values, or values with are only known to be above a certain reporting limit (> laboratory method limit), are less common in environmental datasets but also sometimes present. Particular complexity is added when multiple differing detection limits are present within a single dataset, which is often the case in large environmental monitoring programs which span several decades.

The approach with which these data points are dealt with should not be overlooked. Helsel (2012), for example, has written "the worst practice when dealing with censored observations is to exclude or delete them". Helsel (2012) further strongly discourages the use of simple substitution methods (0, detection limit, or half of the detection limit, for example) in trend analysis. Simple substitution methods can add false signals to the data that were not previously there and can obscure information that is present. This can result in inaccurate and unreproducible results when arbitrary substitution methods are employed. Furthermore, statistical trend detection methods which can be carried out without resorting to the substitution of censored values are well documented and are further detailed in the following sections.

In sections 1.1.1 through 1.1.4, some common methods for handling non-detect values are first explained. These include substitution methods, maximum likelihood estimation, an objective binary method as well as two methods which are commonly used for determining distribution parameters, Kaplan-Meier and regression on order statistics.

2.1.1 Substitution Methods

Previous United States Environmental Protection Agency (USEPA) statistical guidance (USEPA, 2004) had endorsed the use of substituting non-detects with half of the reporting limit when less than 15 % of the samples in a set consisted of non-detects. However, more recent USEPA publications (USEPA, 2013a) do not recommend the use of substitution methods, regardless of how many non-detects are in a sample set. In this USEPA (2013a) document, no particular method for dealing with non-detects is instead provided as a recommendation for trend analyses. For statistical analyses involving the determination of distribution parameters, USEPA (2013a) instead proposes the Kaplan–Meier estimation (KM) or regression on order statistics (ROS) in order to determine distribution parameters of a dataset, both of which cannot meaningfully be applied in trend analysis (See Sect 3.1.4).

Other common substitution methods include replacing all non-detect values by the single highest, lowest or median detection limit or by the value of 0 (Helsel, 2012). The choice of which of these substitution methods to choose has remained subjective. Because of this, modern practices are tending toward avoiding trend analysis methods which require substituted values and instead employing more robust methods, which are capable of preserving censored values.

Substitution methods are, however, still common practise since not all analysis methods are suited for censored data (such as least-squares linear regression or Theil-Sen estimation) or, when analysis methods are suited for censored data, standard commercial software may not be coded to process them. In this case, Helsel (2012) recommends at least first recensoring the dataset at the highest reporting limit – an important step when multiple censoring levels are present in a single set.

2.1.2 Maximum Likelihood Estimation (MLE)

Maximum Likelihood Estimation (MLE) is a parametric approach to handling non-detects (Helsel, 2012). As a parametric approach, using MLE to handle non-detects requires that the data be fitted to a particular distribution. The data thus needs to be checked against a given distribution (normal, lognormal or gamma distribution, for example) before conclusions can be drawn from MLE results.

In MLE, information required consists of: (1) known data points above reporting limits, (2) the proportion of data below each reporting limit and (3) the mathematical formula for an assumed distribution. MLE then computes distribution parameters of (3) to best fit (1) and (2). This method is commonly employed in statistical tests when values of interest are the defining distribution and the distribution parameters of the data, rather than the data points themselves.

2.1.3 Binary Method

Another objective method for handling non-detect data is the binary method. This involves censoring data at the highest detection limit present in the dataset and then classifying each point as either above or below this limit (Helsel, 2012). While it represents some loss of data, this is well suited for a binary logistic regression trend analysis, especially on datasets which contain a high proportion of non-detects.

2.1.4 Kaplan-Meier (KM) and Regression on Order Statistics (ROS)

Other common practices for handling censored values in environmental data come from the field of investigating the distributions of datasets. Particularly, these distributions are used in identifying outlier values or setting threshold limits (often computed by and referred to as "upper confidence limits", or UCL's) at an investigation site. Two of the more commonly employed methods in this field for dealing with non-detects are: the Kaplan–Meier estimation (KM) and regression on order statistics (ROS). These methods are briefly described herein because they are common methods for statistical analyses on environmental data, although neither are applicable for trend analyses.

KM is a method for censored data which is most commonly used in survival analysis. This includes medical studies or failure time studies, where the survival or failure times will often extend beyond the length of the study, resulting in datasets which include right-censored data. It is now also commonly applied to environmental datasets, by fist flipping the dataset by subtracting each data value from a common number which is higher than the highest value in the dataset (so that no negative values result and the dataset becomes right-censored). KM is then carried out by ordering the data and plotting the survival probability percentiles for each distinct value in the set, from which median, mean, variance or other percentile values can be derived.

ROS involves conducting a linear regression on data (or the logarithms of data) versus their normal scores on a probability plot – essentially fitting a normal distribution to the observations (Helsel, 2012). This is carried out on the uncensored observations of a dataset only. From the best-fitting line, mean and variance values can then be determined. Imputed ROS values refer to values which are attributed to censored values in order to accurately compute summary statistics from log-transformed data using ROS, producing "estimated" values for censored data points. In this approach, plotting probabilities for censored values are chosen such that they are evenly-spaced (Helsel, 2012). Helsel (2012) cautions, however, that estimated values should not be assigned to represent any particular censored sample, as there is no valid way of doing so.

While KM and ROS are powerful and common methods for providing summary statistics for datasets, neither of these approaches are well-suited to be applied for trend analyses.

2.2 Environmental Trend Analyses

Trend analysis methods can be classified as either parametric or nonparametric. A method is described as parametric if it assumes that the data belong to a specified probability distribution (often normal or lognormal), which is characterized by defining parameters (e.g. mean and standard deviation) (Ofungwu, 2014). A nonparametric method is an approach which does not require data to belong to any particular distribution, typically relying on relative ranking of data points. Parametric methods in trend analysis include linear regression, while nonparametric methods include Mann-Kendall, Theil-Sen, Spearman's rho and binary logistic regression.

2.2.1 Linear Regression

One of the most widely used techniques in trend detection is linear regression. It is used to relate a response variable (e.g. concentration in mg/l) to one or several explanatory variables (such as time) through a linear model. In linear regression, the traditional least squares method (with substituted censored values) or the MLE method for censored data can be used to estimate the model parameters of slope and intercept. Chung (1990), as well as Thomson and Nelson (2003), have both compared substitution methods (various multiplications of the detection limit and half of the detection limit, respectively) with MLE for regression and found that MLE outperformed substitution methods in estimating model slopes when both were performed on sets containing censored data.

Ofungwu (2014) recommends that linear regression be carried out when at least 8 to 10 data values are present. In MLE, the procedure requires (1) a defining objective function which describes the agreement between the data and the model and (2) a model defined by parameters to be optimized by (1), which attempts to relate y (concentration) to t (time). In a linear model, (2) thus takes the form $y = b_o + b_1 t$, where b_0 and b_1 are the parameters to be optimized by the objective function (1) and y actually refers to the mean (or expected) value of y, which is conditional on t. The objective function is known as the log-likelihood function (L) and is defined by the assumed distribution of the dataset. In MLE, the parameters b_0 and b_1 are optimized such that the likelihood of making the observations, which make up the dataset, is maximized. This method is inherently suited for censored values, as likelihoods can also be determined for censored values with a given distribution.

Using the relationship $y_{expected} = b_o + b_1 t$ for the expected value of the distribution, the log-likelihood function to be maximized can be defined, for normally-distributed residuals containing left-censored data as:

$$L = \sum_{i=1}^{n_d} \log(f(y_i|b_o + b_1\ t_i, \sigma)) + \sum_{i=1}^{n_{nd}} \log(F(y_i|b_o + b_1\ t_i, \sigma))$$

$$+ \sum_{i=1}^{n_{md}} \log(1 - F(y_i|b_o + b_1\ t_i, \sigma)) \qquad (3.1)$$

Where the first term represents the log of the probability given a normal probability density function (f) of making n_d uncensored observations given a mean of $b_o + b_1\ t_i$ and a standard deviation σ, while the second and third terms are the sum of the log of the probabilities based on the cumulative distribution function (F) of making n_{nd} left-censored observations, and n_{md} right-censored observations where the y_i's in this case represent the detection limits. The MLE linear regression method finds the values of b_0, b_1 and σ which maximize the log-likelihood (L). For a lognormal distribution assumption, y values are first log-transformed.

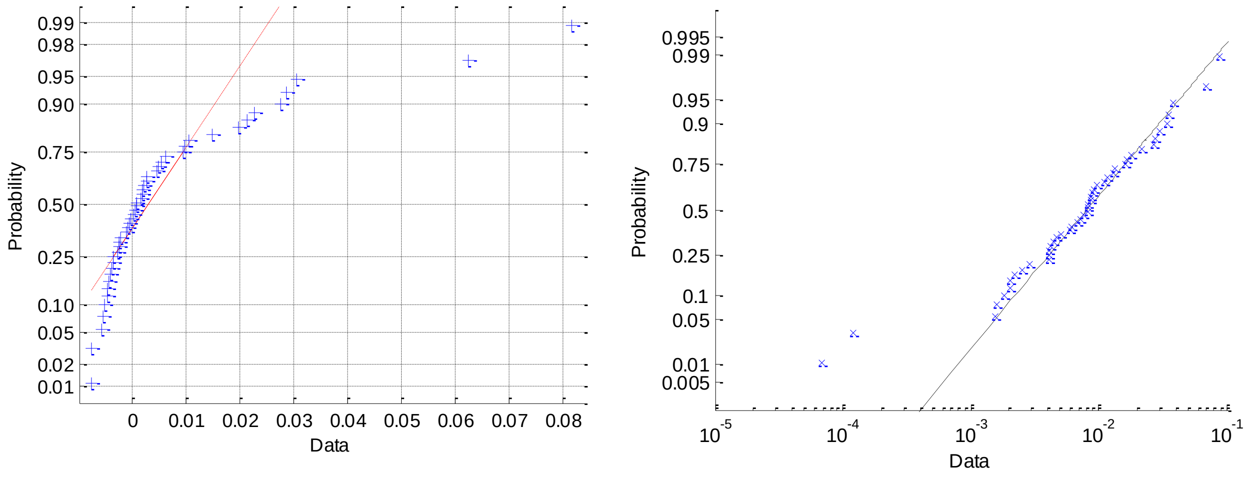
For regression using a gamma distribution assumption on the residuals, the relationship from the gamma distribution of mean = $b_o + b_1\, t_i = k\theta$, where k and θ are the defining shape and scale parameters of the gamma distribution, can be used. Assuming a constant coefficient of variation (cov), the log-likelihood for a gamma distribution on residuals can be derived as:

$$L = \sum_{i=1}^{n_d} \log(p\left(y_i \middle| \frac{1}{cov^2}, cov^2(b_o + b_1\, t_i)\right))$$
$$+ \sum_{i=1}^{n_{nd}} \log(P\left(y_i \middle| \frac{1}{cov^2}, cov^2(b_o + b_1\, t_i)\right))$$
$$+ \sum_{i=1}^{n_{md}} \log(1 - P\left(y_i \middle| \frac{1}{cov^2}, cov^2(b_o + b_1\, t_i)\right)) \tag{3.2}$$

Where $p(y|k,\theta)$ is the probability distribution function of the gamma distribution and $P(y|k,\theta)$ is the cumulative distribution function of the gamma distribution.

Linear regression will provide a representative estimate of model slope and intercept if the following conditions are met: the data are linear, the residuals (distances between observations and fitted model) follow a given distribution and the residuals have a constant variance along the range of the independent variable (Helsel, 2012).

The assumption of the distribution of residuals can be checked once model parameter estimates have been made. Analysis on residuals can be carried out by subtracting the expected value from the observed, for a normal distribution assumption, and by dividing the observed value by the expected, in the case of the lognormal or gamma distribution assumptions. This is done through a probability plot of residuals, such as depicted in Figure 3.1. When the plot of residuals fails to adequately fit the normal distribution assumption, the analysis should be repeated with another distribution assumption (eg. lognormal or gamma). A Chi-square test can also be performed on residuals in order to evaluate the distribution assumption fit.



(a) Normal distribution (b) Lognormal distribution

Figure 2.1 Probability plot (percent of data versus standardized residuals) example from MLE regression estimates with varying distribution assumptions. In this example, the lognormal distribution is better suited for MLE regression of the dataset, though two residual outliers are noted. Crosses represent cummulative probabilities based on observed residuals, lines represent theoretical cummulative probabilities based on the assumed distribution.

In order to test the significance of the computed slope, the maximum log-likelihood obtained from the given model can be compared to the maximum log-likelihood which is obtained without the linear model, in other words, when a slope of 0 is applied (Helsel, 2012). Once log-likelihood values are determined for both the "null model" and the linear model (*L(0)* and *L(b)*, respectively), an overall test statistic (G^2) can be computed by (Helsel, 2012):

$$G^2 = 2(L(b) - L(0)) \tag{3.3}$$

A significance level is then determined by comparing G^2 to a Chi-square distribution with one degree of freedom (Helsel, 2012).

2.2.2 Mann-Kendall

The Mann-Kendall trend test is a nonparametric test which is commonly applied in environmental sciences. The method is also inherently applicable and commonly employed for censored data with a single detection limit and is suited for data which do not meet requirements for a linear regression test. Helsel (2012) also demonstrates how the Mann-Kendall test can be adapted for data with multiple detection limits. However, this capability is seldom coded in most analysis software packages. When multiple detection limit capabilities are not available as part of the analysis in a given software, Helsel (2012) has recommended to first recensor the data at the highest detection limit.

The Mann-Kendall test can be generally considered a test as for whether observed data tend to increase or decrease over time. In addition to being able to handle non-detects and not rely on linearity or normality assumptions, the Mann-Kendall trend test produces reproducible results regardless of whether or not the original data is transformed. The test determines whether, within a specified significance level, the dataset is predominantly increasing, decreasing, or remaining steady over time. It does not, however, produce an estimate of the magnitude of such changes over time. The Mann-Kendall test is computed by first determining the S test statistic as (Helsel and Hirsch, 2002):

$$S = N_c - N_d \tag{3.4}$$

where N_c refers to the number of concordant pairs in a dataset (where the concentration increases as time increases) and N_D refers to the number of disconcordant pairs in a dataset (where the concentration decreases as time increases) and S has properties (Helsel and Hirsch, 2002):

$$E[S] = 0 \tag{3.5}$$

$$Var[S] = \frac{n(n-1)(2n+5)}{18} \tag{3.6}$$

when no data ties are present in a dataset, or (Gilbert, 1987):

$$\begin{aligned} Var[S] = \frac{1}{18}&\{n(n-1)(2n+5) - \textstyle\sum t_i(t_i - 1)(2t_i + 5) - \sum u_i(u_i - 1)(2u_i + 5)\} \\ &+ \frac{1}{9n(n-1)(n-2)}\{\textstyle\sum t_i(t_i - 1)(t_i - 2)\}\{\sum u_i(u_i - 1)(u_i - 2)\} \\ &+ \frac{1}{2n(n-1)}\{\textstyle\sum t_i(t_i - 1)\}\{\sum u_i(u_i - 1)\} \end{aligned}$$

for n observations, in datasets containing ties of extent t_i in the time domain and u_i in the concentration domain. Ties refer here to data pairs (or triplets, etc.) which cannot be considered concordant nor discordant. This refers to, for example, three samples which where taken on the same day (where t=3) or for the tie between the two concentration values <10 and 7, for example (where u=2). When n>10, a normalized Z statistic is then computer as (Helsel and Hirsch, 2002):

$$Z = \begin{cases} \dfrac{S-1}{\sqrt{Var[S]}} & if\ S > 0 \\ 0 & if\ S = 0 \\ \dfrac{S+1}{\sqrt{Var[S]}} & if\ S < 0 \end{cases} \tag{3.7}$$

The test for trend then compares this Z value to the critical, two-tailed test Z value for a given significance level ($Z_{critical}$ = 1.96, for example, for a significance value of 0.05) (Ahmad et al., 2015). A two-tailed test is typically used, as the alternative hypothesis being tested is whether there is either an upward or a downward trend present in the data. If the absolute value of the computed *Z* value is greater than the $Z_{critical}$ value, then the hypothesis that there is no trend is rejected and a trend is said to be identified (increasing for positive S values and decreasing for negative S values).

When $n \leq 10$, the test is performed by finding the exact p value, given S and n, as published by Helsel & Hirsh (2002, Table B8 or Gilbert, 1987 Table A18). It is noted, however, that published p-values for data sets involving ties where $n \leq 10$ are not readily available. In these cases, the use of published tables such as Helsel & Hirsh (2002, Table B8 or Gilbert, 1987 Table A18) would result in inaccuracies.

Mann-Kendall Correction for Autocorrelated Data (Hamed & Rao, 1998)

Hamed & Rao (1998) proposed a correction to the original Mann-Kendall test in order to account for autocorrelation, when it is present in a dataset. The correction involves a modification of the variance to *Var*[S],* such that (Hamed & Rao, 1998):

$$Var^*[S] = Var[S]\frac{n}{n_S^*} \tag{3.8}$$

$$\frac{n}{n_S^*} = 1 + \frac{2}{n(n-1)(n-2)}\ x\ \sum_{i=1}^{n-1}(n-i)(n-i-1)(n-i-2)\rho_s(i) \tag{3.9}$$

where $\rho_s(i)$ is the autocorrelation function of the ranks of the observations and $\frac{n}{n_S^*}$ is a correction factor due to the autocorrelation in the data (Hamed & Rao, 1998). The normalized Z-statistic is then calculated from *Var*[S]* as in the normal Mann-Kendall test. Since data rankings are required, the determination of the autocorrelation function is not inherently suited for datasets which include censoring at multiple levels. Though it results in some loss of data, this can be overcome by recensoring the data at the highest detection limit. Since the correction is carried out on the variance, the correction is only applicable when the normal distribution assumption for the S statistic can be used ($n>10$, or $n \geq 25$ for seasonal Mann-Kendall tests).

Seasonal Mann-Kendall

Environmental data often exhibit seasonal cycles or fluctuations which have been taken into account in the Seasonal Mann-Kendall test, as presented by Hirsch et al. (1982). The Seasonal Mann-Kendall test involves breaking the full dataset into subsets, as categorized by “seasons” (typically months, seasons, or as defined by a sampling interval). The test is recommended when evidence of seasonality exists or is suspected and it is meaningful to test seasonal trends separately. Otherwise, a normal Mann-Kendall test is recommended (Hipel & McLeod, 1994). It is computed similarly to the Mann-Kendall test, where (Helsel & Hirsch, 2002):

$$S_k = \sum_{i=1}^{m} S_i \tag{3.10}$$

$$Var[S_k] = \sum_{i=1}^{m} Var[S_k] \tag{3.11}$$

for m seasons. The selection of a length of a season should be such that there is data available for most of the seasons in record (Helsel & Hirsh, 2002). If samples are collected on a monthly basis, for example, there should be 12 seasons per year and if they are collected quarterly, four (Helsel & Hirsh, 2002). As in the Mann-Kendall test, the Z statistic is then computed and compared to a $Z_{critical}$ value at a specified significance level.

For datasets with an inconsistent sampling interval, Helsel & Hirsch (2002) have recommended that in the case where there are a few instances where no value exists for some season of the year and several samples are available for another season, data can be collapsed into one value per season by taking the median, where applicable. Helsel & Hirsch (2002) then further recommended that, when a systematic change in sampling frequency exists in a dataset, the seasons considered should correspond to the lowest sampling frequency, and the single representative season value should be taken as the value which occurred closest to the mid-point of the season, in order to avoid introducing a trend in the computed variance. Another option in this case, as detailed for the Mann-Kendall test, is to use all values within the same season, but adjust the variance for the ties in the temporal domain (Hipel & McLeod, 1994).

2.2.3 Theil-Sen & Akritas-Theil-Sen Slope Estimation

Theil-Sen type slope estimations are nonparametric methods which, unlike Mann-Kendall tests, produce estimates of the magnitude of slope coefficients. As this test produces an estimate of a single slope coefficient, it is best suited to trends which are approximately linear. When this is not the case, Theil-Sen tests can also be performed on sets of transformed data, such as by using the logarithms of data values (Helsel & Hirsch, 2002). The use of the test also assumes that the trend residuals are independent (Helsel & Hirsch, 2002). USEPA (2009) recommends that this test be carried out when there are at least 10 data values.

In the Theil-Sen test, a slope is computed for every possible data pair, and infinite slopes (for samples collected at the same time) are excluded (USEPA, 2009). The median slope of each pair is then taken as the Theil-Sen slope coefficient. In other words, (Ahmad et al., 2015):

$$T_i = \frac{y_j - y_k}{j - k} \tag{3.12}$$

$$Q = Median\ [T] \tag{3.13}$$

Where y_j and y_k represent data values at times j and k, respectively. Since this computation requires the determination of slopes between all data pairs, this measure is not inherently suited to handle non-detect values. In order to apply this method to a dataset containing non-detects, the use of some substitution method is required.

The Akritas-Theil-Sen is a nonparametric regression method which was developed by Akritas et al. (1995) and is capable of handling censored values without requiring substitution. It has also been shown to outperform Buckley-James regression, commonly used for nonparametric regression of censored data (Helsel, 2012).

In order to compute the Akritas-Theil-Sen slope, first an initial estimate of the slope is set and this is subtracted from the Y (observation) values to create *Y residuals* (where $residual_i = Y_i - slope*X_i$). Kendall's S statistic is then computed between the *Y residuals* and the X variable (time). An iterative search is then conducted to find the slope that will produce an S of zero (Helsel, 2012). Akritas et al. (1995) specifically describe the slope value as the midpoint between the highest known slope which produces a positive S value and the lowest known slope which produces a negative S value. As with the Theil-Sen slope estimator, the Akritas-Theil-Sen method assumes that the data best fit a linear slope model. If this is not the case, the dataset can be transformed prior to analysis.

2.2.4 Spearman's Rho Test

Spearman's rho test is a common nonparametric method for checking whether there is a significant correlation between two variables (Hipel & McLeod, 1994) through a rank-transform. In this test, each variable is ranked separately and Pearson's correlation coefficient (r) is computed for the data ranks (Helsel, 2012). The test is, however, not suitable for datasets with multiple detection limits, since a series of observations such as <1, 3 and <5 cannot be objectively ranked. Helsel (2012), thus recommends first recensoring at the highest detection limit and then assigning the average rank to each of the equivalent values (for example, if four non-detects are present, they are each assigned the rank of 2.5 - the average of ranks 1 through 4). When $R_t^{(X)}$ represents the rank of variable X (time) at time t and $R_t^{(Y)}$ represents the rank of variable Y (concentration) at time t, Spearman's rho is computed by first taking the sum of the squared differences ($S(d^2)$) of the ranks (Hipel & McLeod, 1994):

$$S(d^2) = \sum\left(R_t^{(X)} - R_t^{(Y)}\right)^2 \tag{3.14}$$

and then computing rho (ρ_{XY}) as (Hipel & McLeod, 1994):

$$\rho_{XY} = 1 - \frac{6\,S(d^2)}{n^3 - n} \tag{3.15}$$

when no data ties in X or in Y are present, or (Hipel & McLeod, 1994):

$$\rho_{XY} = \frac{\frac{1}{6}(n^3 - n) - S(d^2) - \frac{1}{12}\Sigma\left(t_j^3 - t_j\right) - \frac{1}{12}\Sigma\left(u_j^3 - u_j\right)}{[\{\frac{1}{6}(n^3 - n) - \frac{1}{6}\Sigma\left(t_j^3 - t_j\right)\}\{\frac{1}{6}(n^3 - n) - \Sigma\left(u_j^3 - u_j\right)\}]^{1/2}} \tag{3.16}$$

for a dataset consisting of n points with t_j and u_j referring to the number of observations in the j^{th} tied group in X and Y, respectively. From ρ_{XY}, a test statistic is computed as (Ahmad et al., 2015):

$$Z = \rho_{XY}\sqrt{\frac{n-2}{1-\rho_{XY}^2}} \tag{3.17}$$

This Z statistic can then be compared to critical values $Z_{critical}$ of the Student's t-distribution with (n-2) degrees of freedom at a specified significance level. If the absolute value of the computed Z value is greater than the $Z_{critical}$ value, then the hypothesis that there is no trend is rejected and a trend is said to be identified (increasing for positive Z values and decreasing for negative Z values).

2.2.5 Binary Logistic Regression

Helsel (2012) has proposed the use of binary logistic regression as an objective and nonparametric method for performing trend analyses on data which contain a high proportion of censored values. Helsel (2012) proposes to first censor all of the data at the highest detection limit present in the dataset and then classifying each observation as binary: either above the detection limit or below it. The logistic regression function is written as (Helsel, 2012):

$$ln\left(\frac{\pi}{1-\pi}\right) = b_o + b_1 t \tag{3.18}$$

where π represents the probability of a concentration being greater than or equal to the detection limit and the left-hand side of the equation is called the logit or logistic transform. The binary logistic regression is then computed using maximum likelihood estimation as in linear regression, where the objective log-likelihood function is now defined by the logistic distribution and parameters b_0 and b_1 are optimized so as to maximize the log-likelihood function. The significance of the regression is then also computed as for linear regression, by comparing the computed maximum log-likelihood to the maximum log-likelihood that is obtained from the logistic distribution without temporal information.

2.2.6 Summary

Due to their common use in environmental analyses and their ability to be adapted to handle non-detect values (as well as non-detects with varied censoring levels), linear regression using MLE, Mann-Kendall, seasonal Mann-Kendall and Theil-Sen/Akritas-Theil-Sen were chosen to be included in the developed software package.

2.3 Existing Software

A wide variety of software targeted to the environmental analysis sector and with trend analysis capabilities is available. Table 3.1 summarizes available software which were reviewed as part of this study. In this software review, particular focus was paid to the programs' characteristics of: input format and flexibility, data pre-processing capabilities (i.e. grouping), trend analysis functions available and flexibility in dealing with non-detect values.

Table 2.1. Selected software available with environmental trend analysis capabilities.

Name	Description & Notes	Pricing
Aquachem By Waterloo Hydrogeologic	Environmental data analysis software package with capabilities including charge balance, sample mixing, descriptive statistics and trend analyses. Flexible input format (text, Excel or Access) and can interface with MODFLOW and PHREEQC. Can compute linear regression, Theil-Sen slope, Mann-Kendall and Seasonal Mann-Kendall tests and Spearman's Rank Correlation. Non-detects set to user-specified fraction of detection limit. Data can be imported from Text, Excel or Access (MSAccess 2000) file.	Commercial Standalone License $1595.00 USD Commercial Team License $2390.50 USD
Chemstat/ Chempoint By Scientific Software Group	Chemstat analysis software works with data management package Chempoint. The software can perform Mann-Kendall Trend tests as well as the Seasonal Kendall, Theil-Sen slope and Spearman's Analyses, but does not support the analysis of multiple wells in a single analysis (a separate script needs to be prepared for analysing multiple wells). User specifies whether non-detects are to be replaced with detection limit, ½ of the detection limit or the value 0 for trend analyses. Data can be imported from data manegement software Chempoint or from Text or Excel files.	Single User License (One Computer $990 USD Upgrade from any previous version (Per-User) $495 USD Associated ChemPoint $390-995 USD
EQuIS By EarthSoft Inc.	Environmental data management software line with GIS integration and sampling planning and processing functions. Includes linear regression, Mann-Kendall and Theil-Sen slope capabilities. Non-detects set to user-specified fraction of detection limit. Data can be imported from Excel or Access.	Single License $~5,000 -10,000 USD, depending on features selected

ESdat By Earth Science Information Systems	Esdat is an environmental data management package which includes functions for sampling pre-planning, mapping, graphing, quality assurance as well as statistical and trend analyses. Data can be imported from a pre-defined Excel file (template provided) and can then be hosted by an Access database or SQL server. ESdat can carry out linear regression as well as Menn-Kendall trend analyses. Non-detects can be set to user-specified fraction of detection limit or replaced by user-specified value.	Single License $~4,800 USD Office-wide License $~14,800 USD
GroundWater Spatiotemporal Data Analysis Tool (GWSDAT) By Shell Global Solutions	This is a free Excel-based program which carries out analysis on groundwater monitoring data and is particularly built to handle data involving the presence of Non-Aqueous Phase Liquids (NAPLs). Statistical functions GWSDAT are carried out in the open programming language R and have the option of being aggregated on a monthly or quarterly time scale. Capabilities of GWSDAT include plotting, mapping, kriging, data visualisation, animation. Trend tests include fitting a linear model to the log of the observations, Mann-Kendall trend test as well as local linear regression (using a smoothing function). User can specifiy to replace non-detects with either half of, or the full detection limit.	Free
Hydro Geoanalyst By Waterloo Hydrogeologic	Hydro GeoAnalyst is an environmental data management, analysis and visualization Software package. (complete data groundwater and borehole environmental data management system). Strengths include 3D data visualization, borehole log plots, ArcGIS integration, animation capabilities and customizable plots. Program also supports user-defined queries and operations on dataset in SQL language. Data can be imported or exported from/to text, Excel or Access files. Trend analysis capabilities, however, are limited to a best-fit line type. Further analysis requires Aquachem extension by Waterloo Hydrogeologic (see Aquachem).	Commercial Standalone License $5995.00 USD Commercial Team License $8992.50 USD
GSI Mann-Kendall Toolkit By GSI Environmental Inc.	Excel spreadsheet for carrying out Mann-Kendall analyses (one parameter at a time) by copying & pasting data into sheet. Non-detects must be substituted by user manually.	Free
MAROS By GSI Environmental Inc.	MAROS is an Access-based program which is intended for data management and analysis. Data can be loaded to MAROS from Excel or Access (chemical names must conform exactly to the nomenclature specified by MAROS format). MAROS has summary statistic capabilities as well as linear regression (on the log of the observations) and Mann-Kendall analysis functions. Non-detects are replaced by half of the detection limit.	Free

ProUCL By US EPA	Developped for the United Stated Environmental Protection Agency to perform parametric and non-parametric statistical analyses. It is a stand-alone Windows application which can import from Excel. Can perform linear regression, Mann-Kendall and Theil-Sen trend tests on idividual wells or well groups. The trend analysis capability of the software, however, is incabable of processing multiple observations within the same sampling period or accept non-detect inputs (user must first substitute non-detect values manually). Time trend capabilities also assume that observation values are entered in a chronological order (program does not read or sort date values).	Free
R Developped by Ross Ihaka and Robert Gentleman, contributers and developpers world-wide	This is a freely available data analysis language with a number of statistical and trend analysis scripts which have been written and are available on the web. In particular, the package EnvStats has been developped specifically for computing statistics in the environmental field. While R is extremely flexible and robust, the learning curve associated with learing the programming language can be steep. See (Millard, 2013), (Chandler & Scott, 2011) and (Bolks et al., 2014) for references regarding using R in environmental trend analysis.	Free
Time trends Niwa	Desktop application can perform Mann-Kendall trend test, Theil-Sen slope estimation, Seasonal Kendall trend test as well as descriptive statistics on one parameter at a time. Non-detects automatically replaced by 0.9 x detection limit, or some user-specified multiple. Can read text, comma delimited or excel files.	Free

In addition to the software listed, analysis is also often done on a fully-customized basis, where programs are developed internally for a company or for particular project. These can be carried out in any number of programming software, such as an Excel or Access Macro, in SQL, R or Matlab. While a large selection of programs for environmental trend analysis is available, it is surprisingly difficult to find a software which is flexible enough to carry out typical environmental trend analysis problems. In many available software, data import formats are non-intuitive and/or conducting a single trend analysis for a project is associated with a steep learning curve.

The program developed within the scope of this project thus hopes to address the available software gap by providing a flexible and user-friendly software which can carry out cited trend analyses (linear regression using MLE, Mann-Kendall, seasonal Mann-Kendall as well as Theil-Sen/Akritas-Theil-Sen) while preserving non-detect data in a meaningful way.

3 Program Implementation

In consideration of the required data inputs, as well as the methods to be implemented and the desired outputs, a conceptual program was developed which involved four separate user interface components. These components are: an initial interface for selecting the project file, an interface for defining relevant data fields, an interface for selecting an analysis and defining its parameters and an interface for displaying the analysis output. These interfaces are further detailed in Figure 5.1.

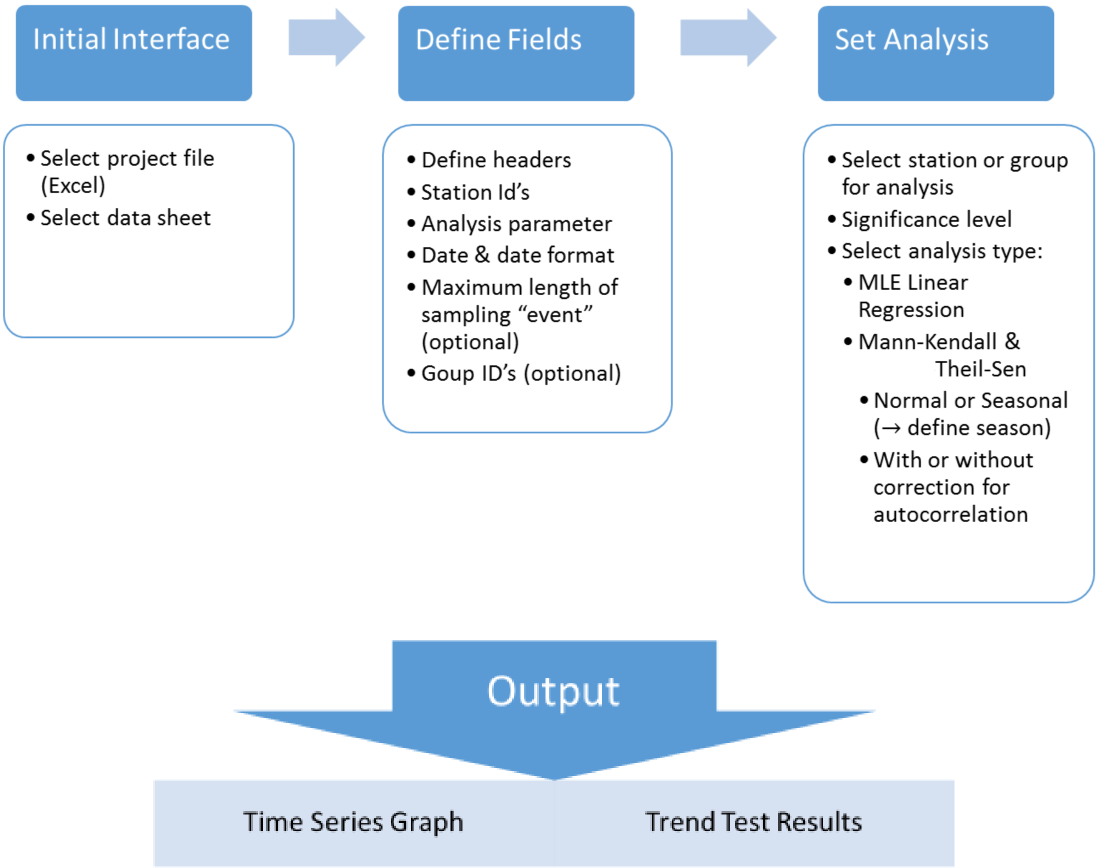


Figure 3.1. Conceptualized program.

Another important consideration in the program development was to ensure that analysis could be repeated quickly and easily after modifying one or several parameters (eg. significance level, test type or station or parameter to be analysed).

In the programming phase of this study project, a program was developed in Matlab2013b in accordance with the conceptual outline and the desired uses of the software. Details regarding the user interfaces are described in the document "User Guide: Literature Review and Software Development for Groundwater and Surface Water Quality Trend Analyses" (2016).

The software was then applied to a case study project, from surface water data collected from the Adige catchment in northern Italy. In the case study, values of ammonium, sulphate, dissolved oxygen, chloride, total phosphorus and conductivity sampled from five stations of the catchment were analysed. Results of this study are discussed and presented in Appendices B and C.

4 Conclusion

Particular challenges face decision-makers when assessing environmental datasets for trends, as these data are rarely well-behaved in fitting an assumed distribution model, may be collected at sporadic or discontinuous intervals, often contain non-detects and can consist of underlying seasonal, autocorrelative as well as stochastic patterns. In the scope of this study project, methods for trend analyses which can address these challenges were researched. The methods of MLE linear regression (using normal, lognormal and gamma distributions) as well as variations of the Mann-Kendall trend test (implemented for seasonal data as well as corrected for data which is autocorrelated) in combination with a determination of Theil-Sen slopes were chosen for implementation in a developed software program, chosen due to their suitability in addressing these environmental dataset challenges.

The software program was then implemented in Matlab 2013b, prepared for user-suitability and flexibility and then packaged for distribution. Finally, a case study on ammonium, sulphate, dissolved oxygen, chloride, total phosphorus and conductivity data collected from five stations on the Adige catchment was successfully carried out using the software (Appendix B-C).

Further development in the direction of this study project could be aimed at adding additional features to the developed software. While the program developed is well-equipped to process observations which are below some detection threshold, capabilities for processing values which are above quantification limits (eg. >50) have not been addressed. Such capabilities would be recommended to integrate into the software as a next improvement. Since it is desirable for users to be able to perform a variety of trend analysis approach methods, future developments could examine also implementing binary logistic regression as well as Spearman's Rho test.

In the Adige case study, trend analysis results were able to demonstrate how users can be provided with additional and stronger evidence to support decision-making by carrying out a variety of approaches and analysis methods. These capabilities have been made available in the software developped for this study project. Further details regarding methods implemented as well as limitations of the program developped are described in the document "User Guide: Literature Review and Software Development for Groundwater and Surface Water Quality Trend Analyses" (2016).

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Appendix B: Adige Catchment Case Study

Introduction

Following program implementation and debugging, a case study analysis was carried out on data available from the Adige river catchment. The dataset consisted of observations of routine parameters, nutrients, metals and common pesticides available from a total of 70 stations in the catchment network. The river network has an extremely low (almost 0) detection history of metals of concern and pesticides. For the purpose of the case study, data from five stations were examined for trends in concentrations of ammonium (NH_4^+), sulphate (SO_4^{2-}), dissolved oxygen (DO), chloride (Cl^-), total phosporus (P) and conductivity. The stations examined were (Figure B.1):

- FIUME ADIGE Ponte San Lorenzo (2004-2013)
- FIUME ADIGE Ponte di Mattarello (2004-2008)
- FIUME AVISIO Lavis (2004-2013)
- TORRENTE NOCE loc. Rupe (2004-2013)
- TORRENTE NOCE Ponte di Cavizzana (2004-2013)

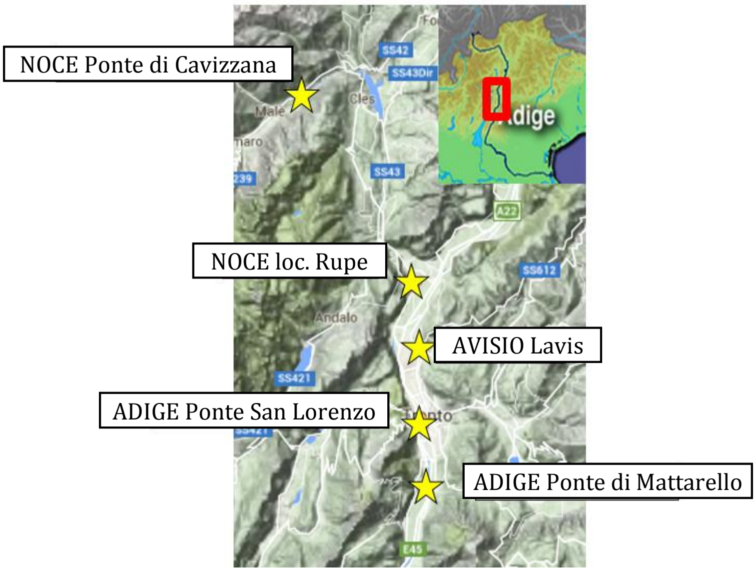


Figure B.1 Locations of stations analysed from the Adige catchment (Google Maps, 2016).

Data from these stations were collected between 2004 and 2013 (2004-2008 at the station FIUME ADIGE Ponte di Mattarello) at a frequency of approximately monthly. Time series graphs for stations and parameters analysed are provided in Appendix B. For each parameter at each station, MLE linear regression results are reported for the distribution which represented the best fit of the dataset, as reported by the Chi-square test on the residuals. Where all of the distributions were rejected by the Chi-square test (at a significance <0.05), no linear regression analysis result is displayed. Further details regarding data processing in the developed software, refer to document

"User Guide: Literature Review and Software Development for Groundwater and Surface Water Quality Trend Analyses" (2016).

Mann-Kendall as well as seasonal Mann-Kendall tests were also performed on each of the datasets. The seasonal test was performed on twelve seasons per year, since data was collected approximately monthly. Estimated Akritas-Theil-Sen lines are, however, presented for simplicity on a seasonal basis at four per year. They have been thus presented for conciseness (and to avoid "data overload") and are herein presented for general discussion. Where significant correlation was detected in the dataset, corrected p-values on the Mann-Kendall trend tests are reported.

Ammonium (NH_4^+)

MLE linear regression as well as Mann-Kendall trend analysis results for ammonium at the five reference stations are presented in Table B.1 and Appendix C-1. In the linear regression of all of the five stations, negative trends were identified at the stations Adige-Ponte San Lorenzo as well as at Noce-Ponte di Cavizzana. None of the stations reported a trend as a result of the general Mann-Kendall test. However, a seasonal pattern was evident in the ammonium datasets and the stations Adige-Ponte San Lorenzo as well as at Noce-Ponte di Cavizzana also both reported negative trends when the seasonal Mann-Kendall test was implemented. An additional negative trend was identified by the seasonal Mann-Kendall trend test at Noce-loc. Rupe, though the Akritas-Theil-Sen slopes for this station were near 0.

Table B.1 Ammonium: Adige catchment trend analysis case study results.

		FIUME ADIGE Ponte San Lorenzo	FIUME ADIGE Ponte di Mattarello	FIUME AVISIO Lavis	TORRENTE NOCE loc. Rupe	TORRENTE NOCE Ponte di Cavizzana
# of Observations	Total	120	32	120	120	120
	Non-Detects	9	2	67	58	13
MLE Linear Regression	Best Fit Dist.	Lognormal (p: 0.56)	Lognormal (p: 0.68)	Lognormal (p: 0.22)	Lognormal (p: 0.11)	Lognormal (p: 0.14)
	Trend p	**0.038**	0.43	0.83	0.13	**0.01**
	Slope	**-3.9%/y**	-	-	-	**-5.7%/y**
Mann-Kendall	p	0.23(corr*)	0.96	0.99	0.12	0.078(corr*)
	Theil-Sen	-	-	-	-	-
Seasonal Mann-Kendall	$p_{12\ seasons/year}$	**<1e-6 (decreasing)**	0.65	0.96	**0.047 (decreasing)**	**<1e-6 (decreasing)**
	Akritas-Theil-Sen_{Winter}	-0.0025 mg/l·y	-	-	<1e-6	-0.0067 mg/l·y
	Akritas-Theil-Sen_{Spring}	-0.0021 mg/l·y	-	-	<1e-6	-0.0033 mg/l·y
	Akritas-Theil-Sen_{Summer}	<1e-6	-	-	<1e-6	<1e-6
	Akritas-Theil-Sen_{Fall}	-0.0025 mg/l·y	-	-	<1e-6	-0.0017 mg/l·y

*corr: Autocorrelation present in dataset, p-value represents p-value corrected for autocorrelation.

Sulphate (SO_4^{2-})

In the linear regression of sulphate concentrations at each of the five stations, either no significant trend in concentrations was detected from the regression or the residual analysis concluded that none of the assumed distributions provided an appropriate fit for the data (Table B.2). Again, none of the stations reported a trend as a result of the general Mann-Kendall test. Although a strong seasonal pattern was evident in the sulphate datasets, none of the stations reported a significant trend as a result of the seasonal Mann-Kendall test.

Table B.2 Sulphate: Adige catchment trend analysis case study results.

		FIUME ADIGE Ponte San Lorenzo	FIUME ADIGE Ponte di Mattarello	FIUME AVISIO Lavis	TORRENTE NOCE loc. Rupe	TORRENTE NOCE Ponte di Cavizzana
# of Observations	Total	120	32	120	120	120
	Non-Detects	0	0	0	0	0
MLE Linear Regression	Best Fit Dist.	Lognormal (p: 0.39)	Gamma (p: 0.12)	Normal (p: 0.81)	None (Normal best, rejected at p: 0.012)	None (Lognormal and Gamma best, rejected at p: 0.034)
	Trend p	0.54	0.70	0.61	-	-
	Slope	-	-	-	-	-
Mann-Kendall	p	0.65	0.50	0.60(corr*)	0.98(corr*)	0.11(corr*)
	Theil-Sen	-	-	-	-	-
Seasonal Mann-Kendall	$p_{12\ seasons/year}$	0.29	1.00	0.58	0.43	0.13(corr*)
	Akritas-Theil-Sen_{Winter}	-	-	-	-	-
	Akritas-Theil-Sen_{Spring}	-	-	-	-	-
	Akritas-Theil-Sen_{Summer}	-	-	-	-	-
	Akritas-Theil-Sen_{Fall}	-	-	-	-	-

*corr: Autocorrelation present in dataset, p-value represents p-value corrected for autocorrelation.

Dissolved Oxygen (DO)

In the linear regression of all of the five stations, the dissolved oxygen (DO) residuals were found to be best modelled by either the lognormal or gamma distribution (Table B.3 & Appendix C-2). The stations Noce-loc. Rupe as well as Noce-Ponte di Cavizzana were found to both have significant negative trends in DO as per the linear regression analysis. These negative trends were further captured by the Mann-Kendall test for the station Ponte di Cavizzana and by the seasonal Mann-Kendall test at both of these stations. At the station Avisio-Lavis, a decreasing trend was also identified by the seasonal Mann-Kendall test, which had not been identified by linear regression or by the traditional Mann-Kendall test.

Table B.3 Dissolved oxygen: Adige catchment trend analysis case study results.

		FIUME ADIGE Ponte San Lorenzo	FIUME ADIGE Ponte di Mattarello	FIUME AVISIO Lavis	TORRENTE NOCE loc. Rupe	TORRENTE NOCE Ponte di Cavizzana
# of Observations	Total	120	43	120	120	120
	Non-Detects	0	0	0	0	0
MLE Linear Regression	Best Fit Dist.	None (Lognormal best, rejected at p: 0.0049)	Gamma (p: 0.13)	Lognormal (p: 0.42)	Gamma (p: 0.97)	Lognormal (p: 0.98)
	Trend p	-	0.99	0.24	**0.0025**	**0.034**
	Slope	-	-	-	**- 0.11 mg/l·y**	**- 0.58 %/y**
Mann-Kendall	p	0.40(corr*)	1.00	0.20 (corr*)	0.095 (corr*)	**0.027 (corr*) (decreasing)**
	Theil-Sen	-	-	-	-	- 0.068 mg/l·y
Seasonal Mann-Kendall	$p_{12\ seasons/year}$	0.077(corr*)	0.057	**0.032 (decreasing)**	**0.00096(corr*) (decreasing)**	**0.00053 (decreasing)**
	Akritas-Theil-Sen_{Winter}	-	-	-0.018 mg/l·y	-0.080 mg/l·y	-0.10 mg/l·y
	Akritas-Theil-Sen_{Spring}	-	-	-0.018 mg/l·y	-0.15 mg/l·y	-0.038 mg/l·y
	Akritas-Theil-Sen_{Summer}	-	-	-0.075 mg/l·y	-0.033 mg/l·y	-0.14 mg/l·y
	Akritas-Theil-Sen_{Fall}	-	-	-0.069 mg/l·y	-0.075 mg/l·y	-0.059 mg/l·y

*corr: Autocorrelation present in dataset, p-value represents p-value corrected for autocorrelation.

Chloride (Cl^-)

MLE linear regression as well as Mann-Kendall trend analysis results for chloride at the five reference stations are presented in Table B.4 and Appendix C-3. At the station Noce-loc. Rupe, linear regression indicated a significant negative trend in chloride concentrations. This was further identified by the seasonal Mann-Kendall test. The seasonal Mann-Kendall test further detected a significant positive trend in chloride concentrations at Avisio-Lavis (strongest in the winter observations), but this could not be supported by linear regression results since the dataset failed to adequately fit any of the distributions tested.

Table B.4 Chloride: Adige catchment trend analysis case study results.

		FIUME ADIGE Ponte San Lorenzo	FIUME ADIGE Ponte di Mattarello	FIUME AVISIO Lavis	TORRENTE NOCE loc. Rupe	TORRENTE NOCE Ponte di Cavizzana
# of Observations	Total	120	32	120	120	120
	Non-Detects	0	0	0	0	0
MLE Linear Regression	Best Fit Dist.	Lognormal (p: 0.091)	Gamma (p: 0.37)	None (Lognormal best, rejected at p: 2.2e-5)	Lognormal (p: 0.46)	None (Lognormal best, rejected at p: 0.016)
	Trend p	0.71	0.93	-	**0.039**	-
	Slope	-	-	-	**-2.4 %/y**	-
Mann-Kendall	p	0.59 (corr*)	0.51(corr*)	0.44 (corr*)	0. 27 (corr*)	0.60 (corr*)
	Theil-Sen	-	-	-	-	-
Seasonal Mann-Kendall	$p_{12\ seasons/year}$	0.095(corr*)	0.33	**0.013 (increasing)**	**0.034 (decreasing)**	0.17 (corr*)
	Akritas-Theil-Sen_{Winter}	-	-	0.31 mg/l·y	<1e-6	-
	Akritas-Theil-Sen_{Spring}	-	-	-0.71 mg/l·y	-0.088 mg/l·y	-
	Akritas-Theil-Sen_{Summer}	-	-	0.10 mg/l·y	-0.050 mg/l·y	-
	Akritas-Theil-Sen_{Fall}	-	-	0.020 mg/l·y	-0.050 mg/l·y	-

*corr: Autocorrelation present in dataset, p-value represents p-value corrected for autocorrelation.

Total Phosphorus (P)

In the linear regression analysis, two out of the five phosphorus datasets at the stations examined failed to fit any of the modelled distribution assumptions (Table B.5 & Appendix C-4). At Adige-Ponte San Lorenzo, however, the lognormal distribution assumption could not be rejected and a negative trend was identified. The general Mann-Kendall test also reported a significant negative trend at this station as well as at Noce-loc. Rupe (although the Theil-Sen slope was computed as 0). In the seasonal Mann-Kendall test, negative trends were reported for Adige-Ponte San Lorenzo and Noce-Ponte di Cavizzana. At these stations, the negative trends were strongest in the summer months.

Table B.5 Total Phosphorus: Adige catchment trend analysis case study results.

		FIUME ADIGE Ponte San Lorenzo	FIUME ADIGE Ponte di Mattarello	FIUME AVISIO Lavis	TORRENTE NOCE loc. Rupe	TORRENTE NOCE Ponte di Cavizzana
# of Observations	Total	120	32	120	120	120
	Non-Detects	0	0	5	1	0
MLE Linear Regression	Best Fit Dist.	Lognormal (p: 0.32)	Lognormal (p: 0.12)	None (Gamma best, rejected at p: 0.012)	None (Gamma best, rejected at p: 0.0015)	Lognormal (p: 0.074)
	Trend p	**0.01**	0.45	-	-	0.098
	Slope	**-3.4%/y**	-	-	-	-
Mann-Kendall	p	**0.019 (corr*) (negative)**	0.25	0.79 (corr*)	**0.033 (negative)**	0.13 (corr*)
	Theil-Sen	-0.0012	-	-	<1e-6	-
Seasonal Mann-Kendall	$p_{12\ seasons/year}$	**<1e-6 (negative)**	0.59	1.0	0.17	**1.2e-5 (corr*) (negative)**
	Akritas-Theil-Sen_{Winter}	-0.0013 mg/l·y	-	-	-	<1e-6
	Akritas-Theil-Sen_{Spring}	<1e-6	-	-	-	<1e-6
	Akritas-Theil-Sen_{Summer}	-0.0025 mg/l·y	-	-	-	-0.0018 mg/l·y
	Akritas-Theil-Sen_{Fall}	-0.0017 mg/l·y	-	-	-	<1e-6

*corr: Autocorrelation present in dataset, p-value represents p-value corrected for autocorrelation.

Conductivity

In the linear regression of conductivity at each of the five stations, either no significant trend in concentrations was detected from the regression or the residual analysis concluded that none of the assumed distributions provided an appropriate fit for the data (Table B.6 & Appendix C-5). The general Mann-Kendall test also failed to identify any trends, however, a seasonal pattern was evident in the datasets. The seasonal Mann-Kendall test detected a significant negative trend in the conductivity values at Adige-Ponte San Lorenzo, which was particularly stronger in the winter and spring observations.

Table B.6 Conductivity: Adige catchment trend analysis case study results.

		FIUME ADIGE Ponte San Lorenzo	FIUME ADIGE Ponte di Mattarello	FIUME AVISIO Lavis	TORRENTE NOCE loc. Rupe	TORRENTE NOCE Ponte di Cavizzana
# of Observations	Total	120	32	120	120	120
	Non-Detects	0	0	0	0	0
MLE Linear Regression	Best Fit Dist.	Lognormal (p: 0.076)	Lognormal (p: 0.22)	Normal (p: 0.59)	Normal (0.33)	None (Lognormal best at p: 0.033)
	Trend p	0.17	0.66	0.098	0.37	-
	Slope	-	-	-	-	-
Mann-Kendall	p	0.16 (corr*)	0.71 (corr*)	0.44 (corr*)	0.61 (corr*)	0.55 (corr*)
	Theil-Sen	-	-	-	-	-
Seasonal Mann-Kendall	$p_{12\ seasons/year}$	**0.014 (negative)**	0.099	0.11	0.41	0.34
	Akritas-Theil-Sen_{Winter}	-2.7 µS/cm·year	-	-	-	-
	Akritas-Theil-Sen_{Spring}	-3.2 µS/cm·year	-	-	-	-
	Akritas-Theil-Sen_{Summer}	0.22 µS/cm·year	-	-	-	-
	Akritas-Theil-Sen_{Fall}	-1.3 µS/cm·year	-	-	-	-

*corr: Autocorrelation present in dataset, p-value represents p-value corrected for autocorrelation.

Case Study Summary

In the analyses conducted on the selected stations of the Adige catchment, it was found in the MLE linear regression assessment that these water quality datasets were not always well-behaved with respect to fitting any particular distribution model. The residuals of many of the sets failed to fit either the normal, lognormal or gamma distribution. Of the ones which did fit, the lognormal distribution most often provided the best fit of the residuals. A normal distribution of residuals provided a best fit in 3 cases, a gamma distribution in 4 cases, and a lognormal distribution in 15 cases. In 8 cases, all three of the distributions tested were rejected by the Chi-square goodness-of-fit test.

Seasonal patterns appeared to be present in each of the parameters (ammonium, sulphate, dissolved oxygen, chloride, total phosphorus and conductivity) which were analysed, suggesting that the use of a seasonal Mann-Kendall trend test would be more appropriate for such data, which was collected monthly for these parameters. Trends detected by the seasonal Mann-Kendall test (at a significance level of 0.05) consisted of:

- Ammonium: Decreasing trends at Adige-Ponte San Lorenzo, Noce-loc. Rupe and Noce-Ponte di Cavizzana
- Dissolved oxygen: Decreasing trends at Avisio-Lavis, Noce-loc. Rupe and Noce-Ponte di Cavizzana
- Chloride: Increasing trend at Avisio-Lavis, particularly in winter observations, and decreasing trend at Noce-loc. Rupe, particularly in spring, summer and fall
- Total Phosphorus: Decreasing trends at Adige-Ponte San Lorenzo and Noce-Ponte di Cavizzana, particularly in summer observations
- Conductivity: Decreasing trend at Adige-Ponte San Lorenzo, particularly in winter and spring observations

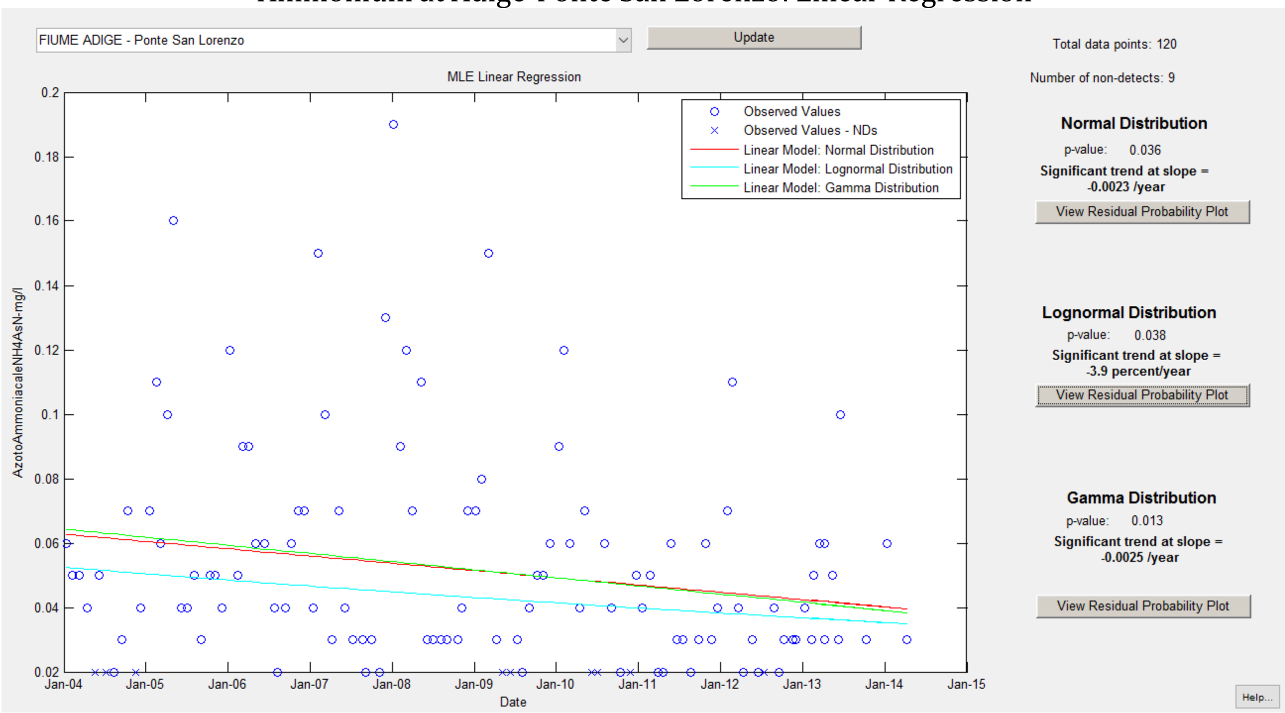
When a fit was adequate, the linear regression test conclusion (presence and direction of trend) agreed with the general Mann-Kendall test conclusion in 18 out of 23 cases, providing additional evidence to support trend conclusions. The seasonal Mann-Kendall analysis results agreed with the linear regression results in 19 out of 23 cases.

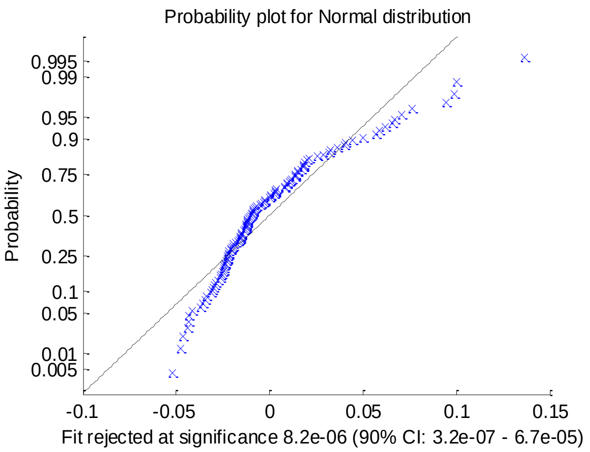
In examining the probability plots and Chi-square results on the residuals of linear regressions for data containing non-detects, it was observed that a very wide range of p-values could result from randomized trials of the Chi-square test (as ouputted as 90% interval, often spanning orders of magnitude at smaller values) when various values between 0 and the detection limit were substituted for non-detects in the residual analyses. This goodness-of-fit evaluation can thus be extremely sensitive to how non-detects are treated. An approach which evaluates 1000 trials using the assumed distribution is thus built-in to the developped software, outputting both the median value as well a range containing the mid-90% of the results from the goodness-of-fit evaluations.

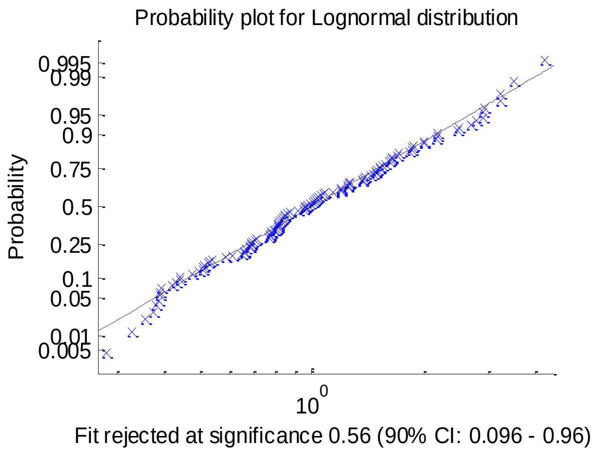
In implementing Mann-Kendall analysis in combination with a determination of the Akritas-Theil-Sen slope, it was observed that, in some cases, an either increasing or decreasing Mann-Kendall trend can be identified at a significance level of 0.05, however, the reported Theil-Sen slope could be 0. This is especially likely in datasets which contain seasonal patterns as well as a large number of equivalent observations. This further highlights the weaknesses associated with using these methods on their own and the importance of objectively examining results from a variety of methods before conclusions can be drawn. This case study has exhibited how users can be provided with additional and stronger evidence to support decision-making by carrying out a variety of approaches and analysis methods.

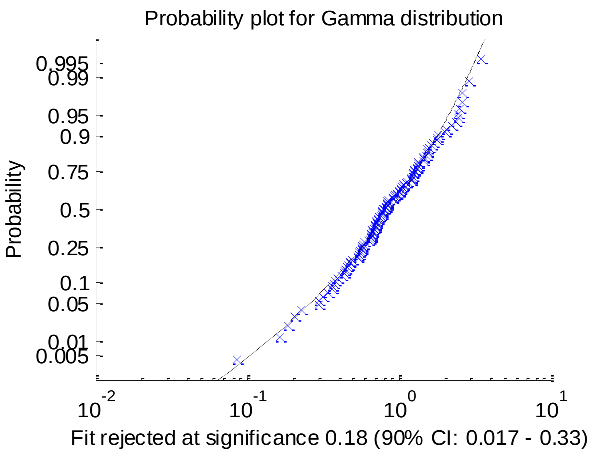
Appendix C-1: Adige Catchment Trend Analysis Case Study Results – Ammonium

Ammonium at Adige-Ponte San Lorenzo: Linear Regression

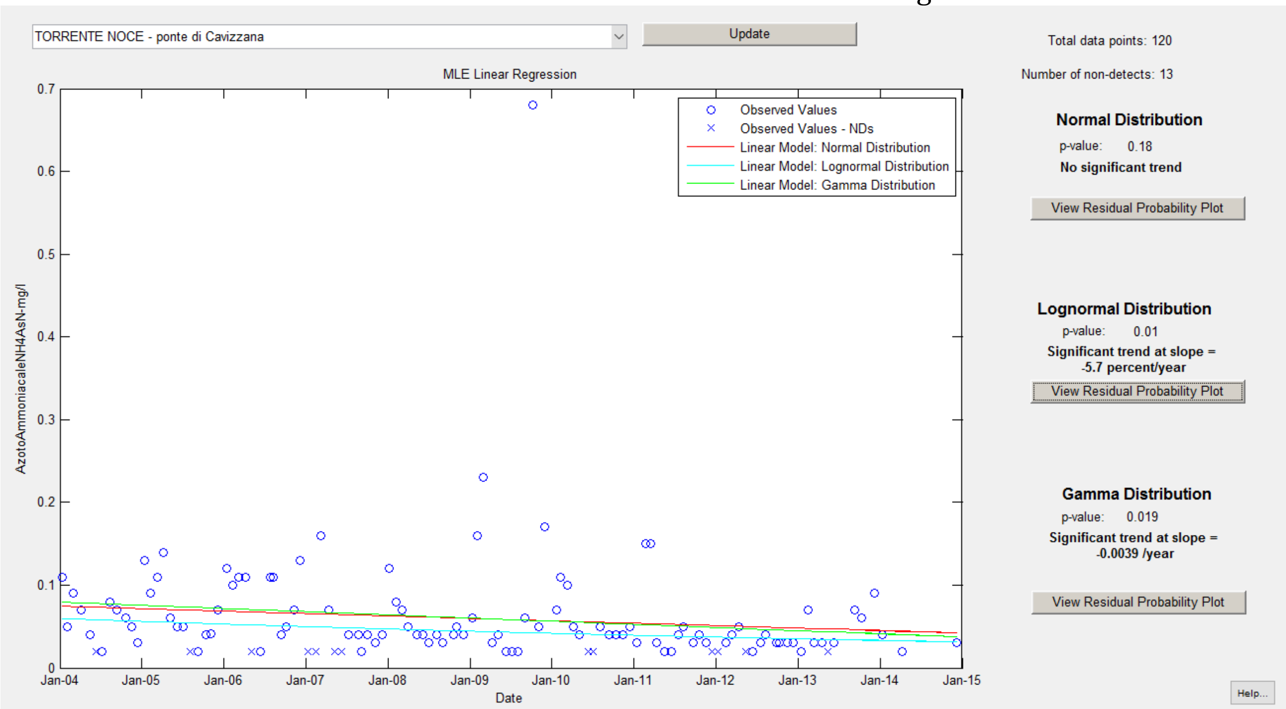




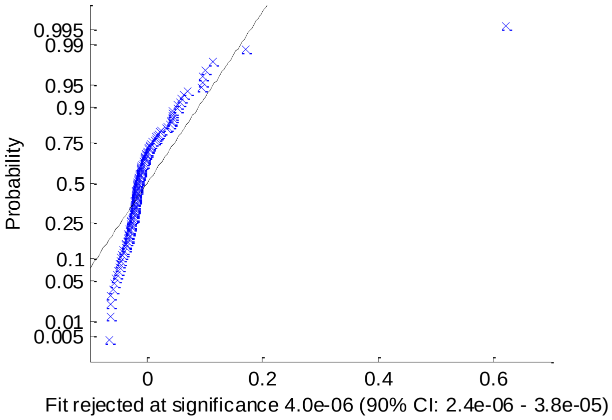




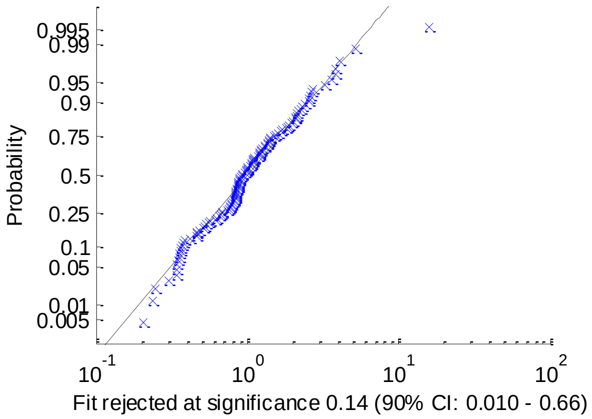
Ammonium at Noce-Ponte di Cavizzana: Linear Regression



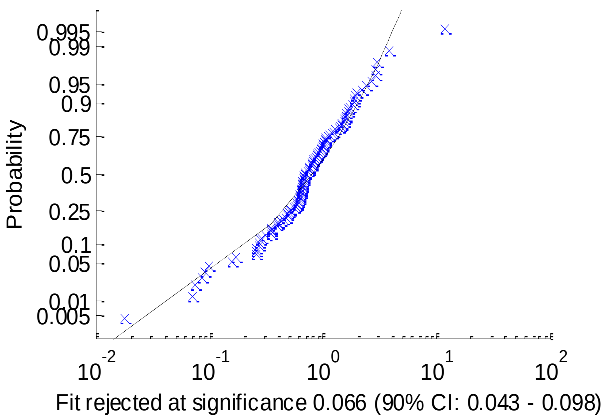
Probability plot for Normal distribution



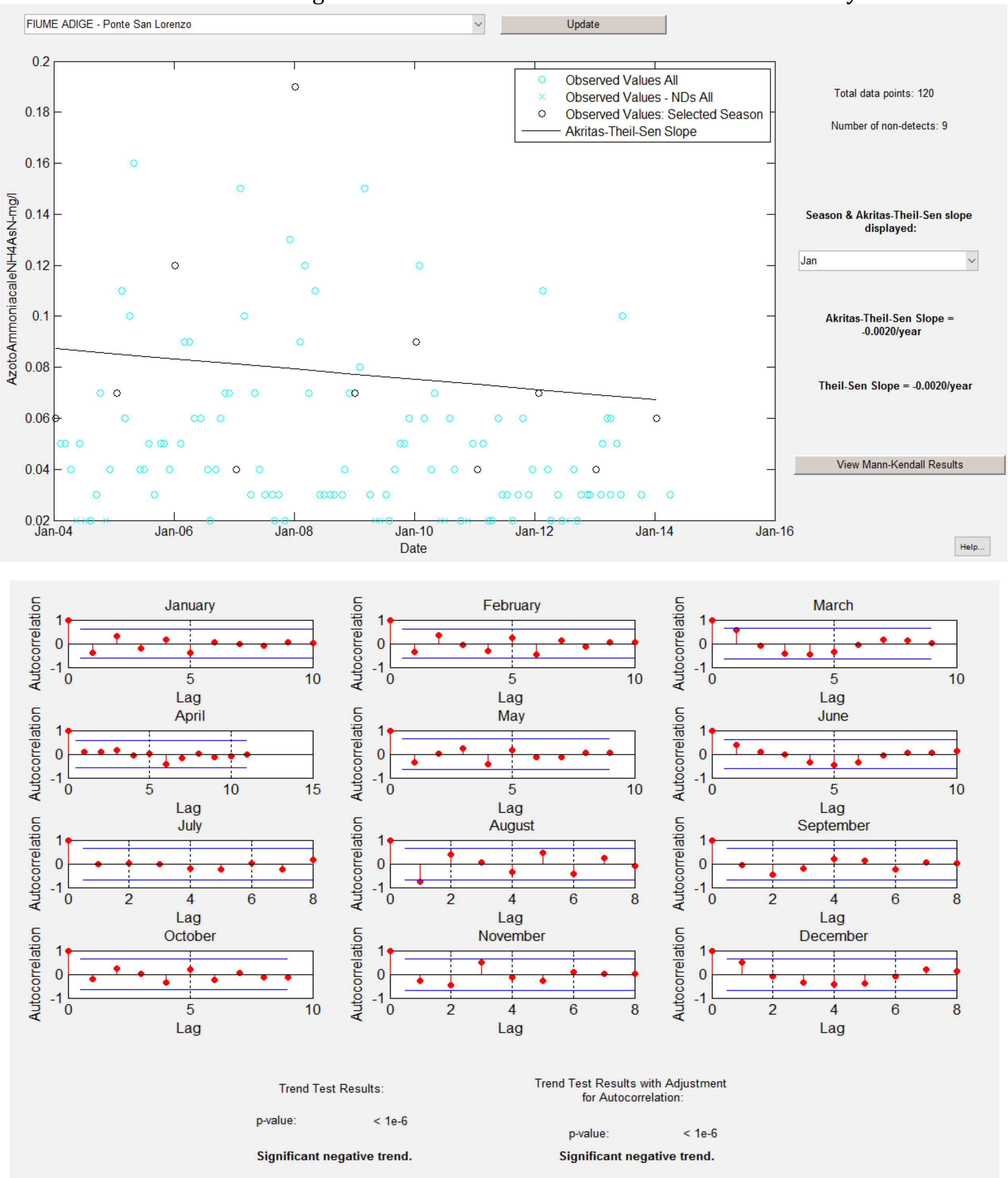
Probability plot for Lognormal distribution



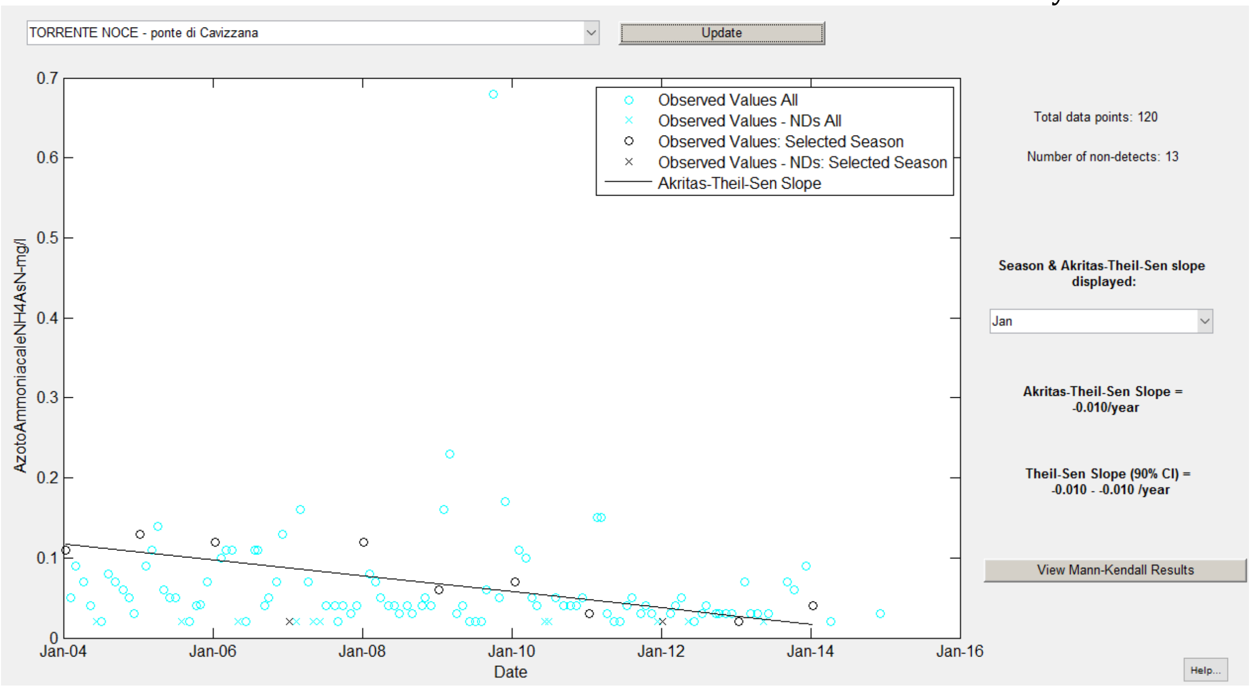
Probability plot for Gamma distribution

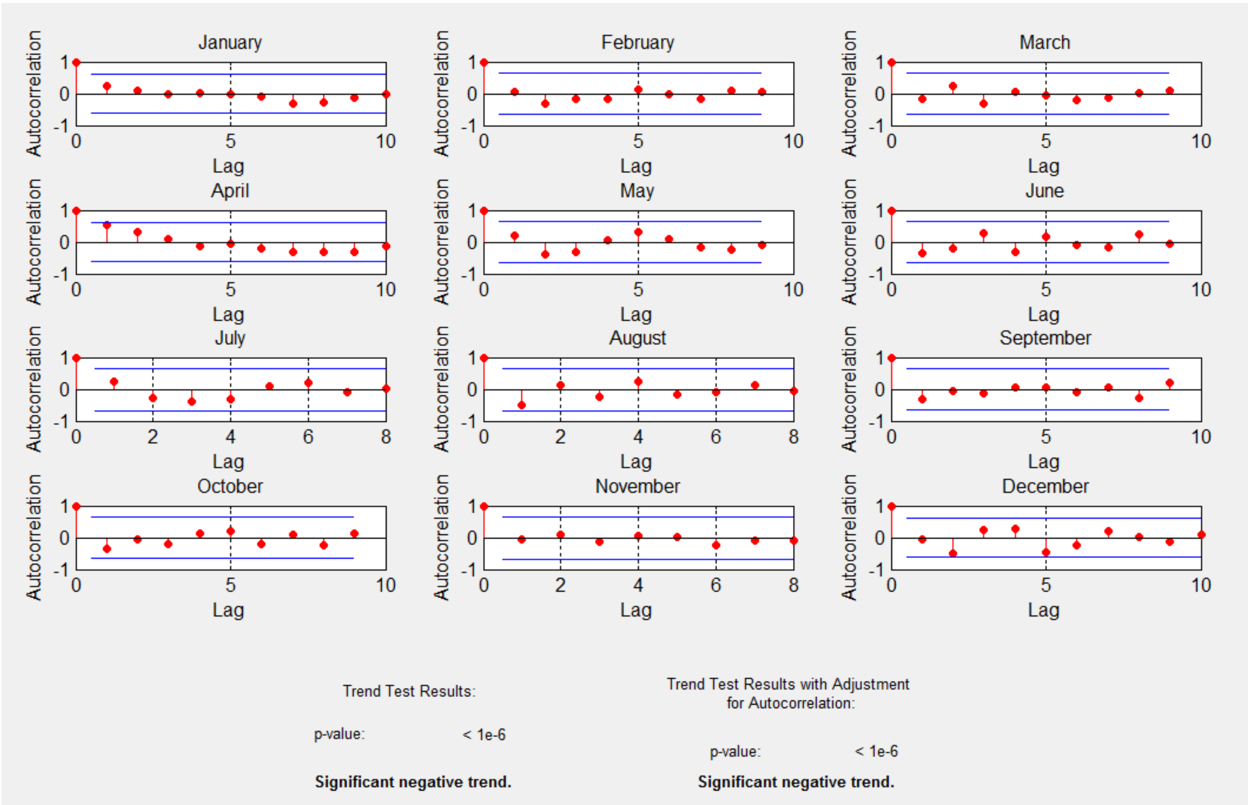


Ammonium at Adige-Ponte San Lorenzo: Seasonal Mann-Kendall Analysis



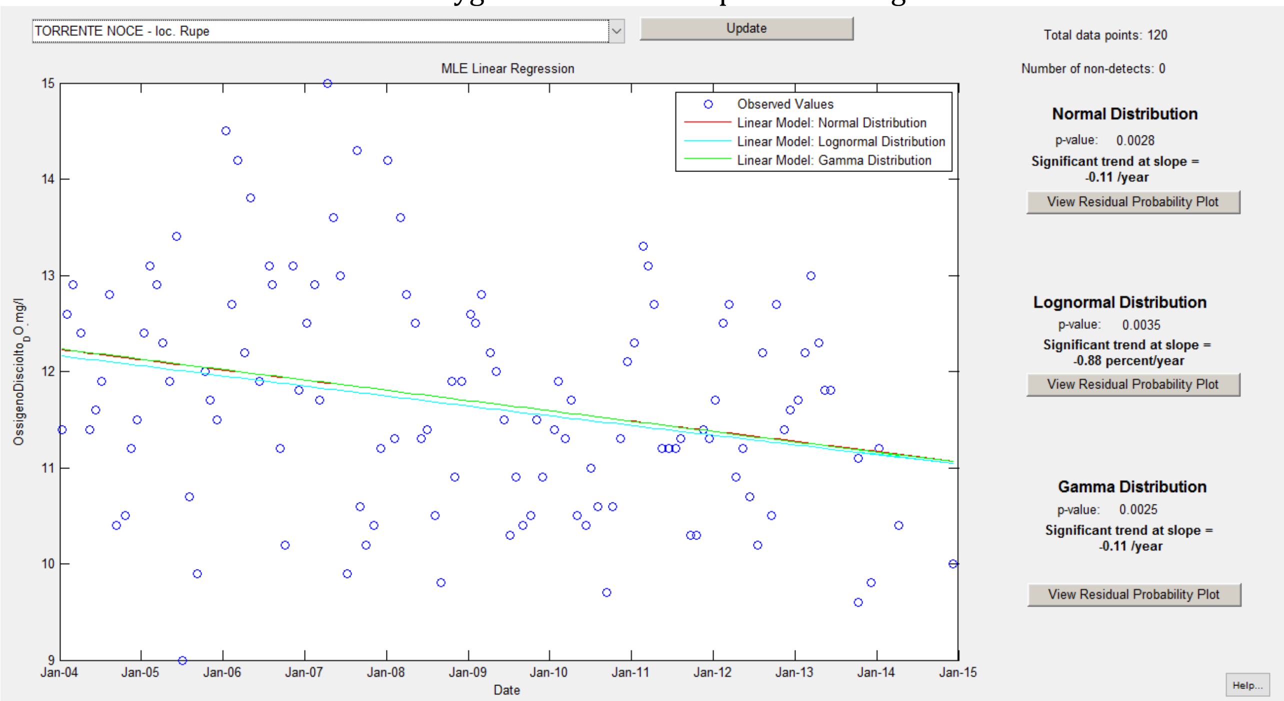
Ammonium at Noce-Ponte di Cavizzana: Seasonal Mann-Kendall Analysis

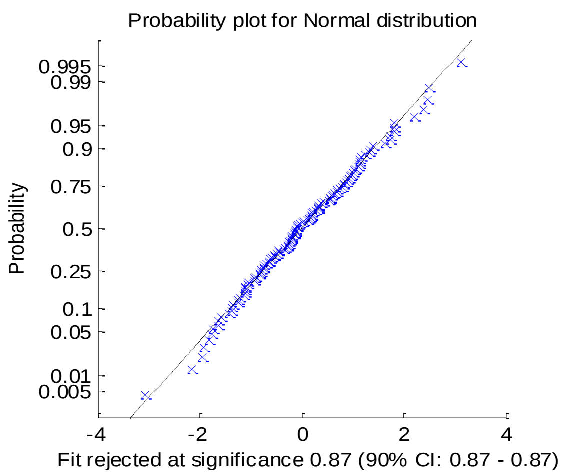


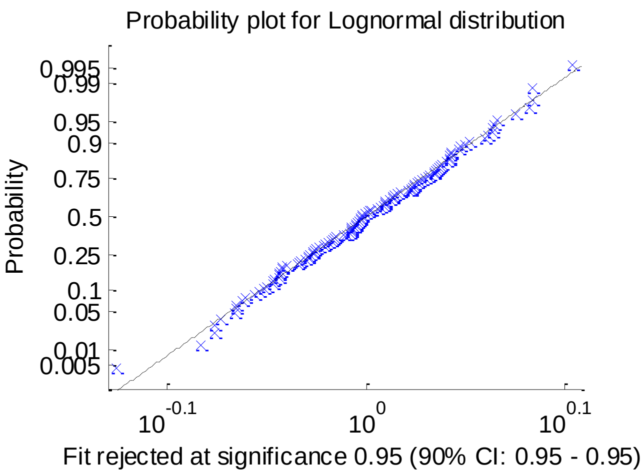


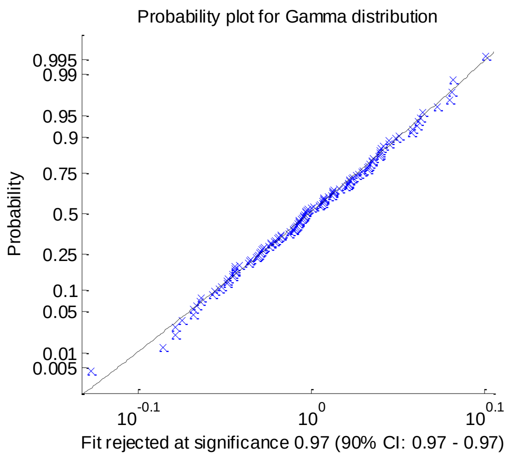
Appendix C-2: Adige Catchment Trend Analysis Case Study Results – Dissolved Oxygen

Dissolved Oxygen at Noce-loc. Rupe: Linear Regression

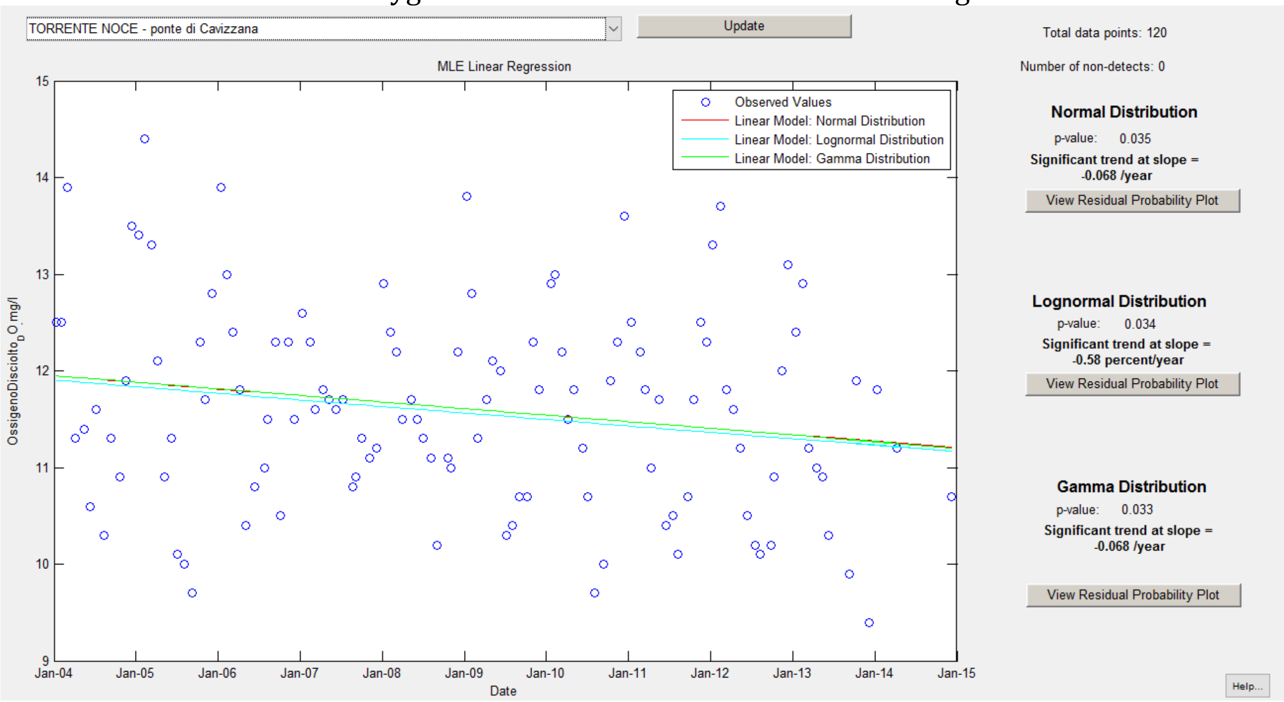


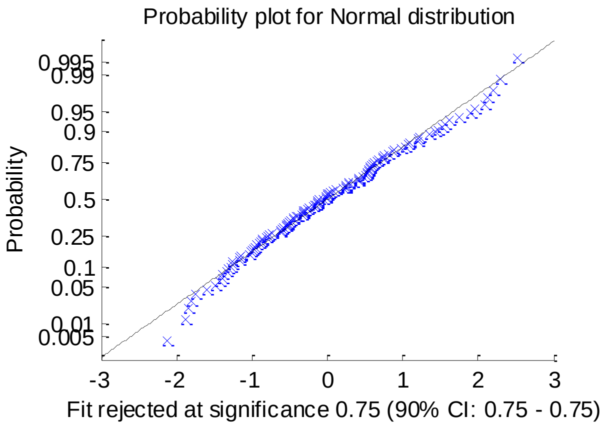


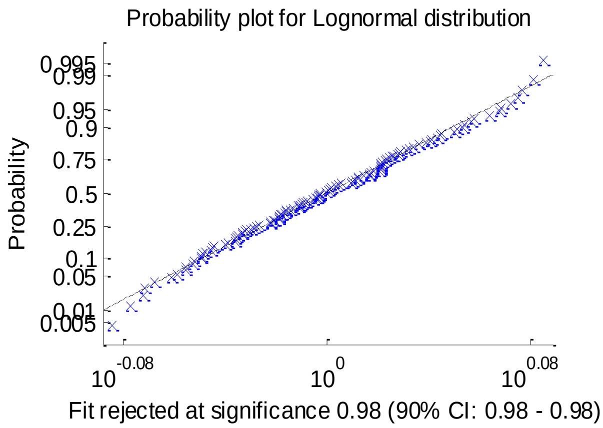


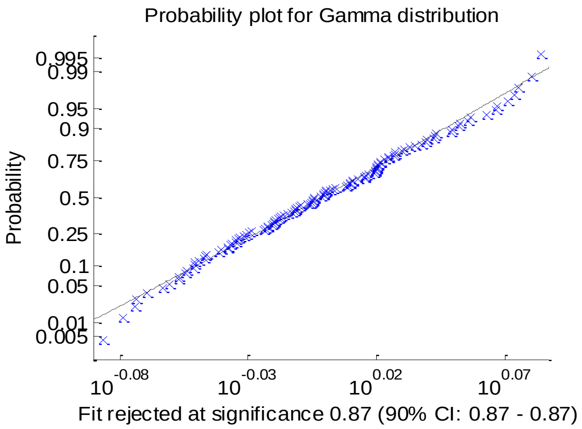


Dissolved Oxygen at Noce-Ponte di Cavizzana: Linear Regression

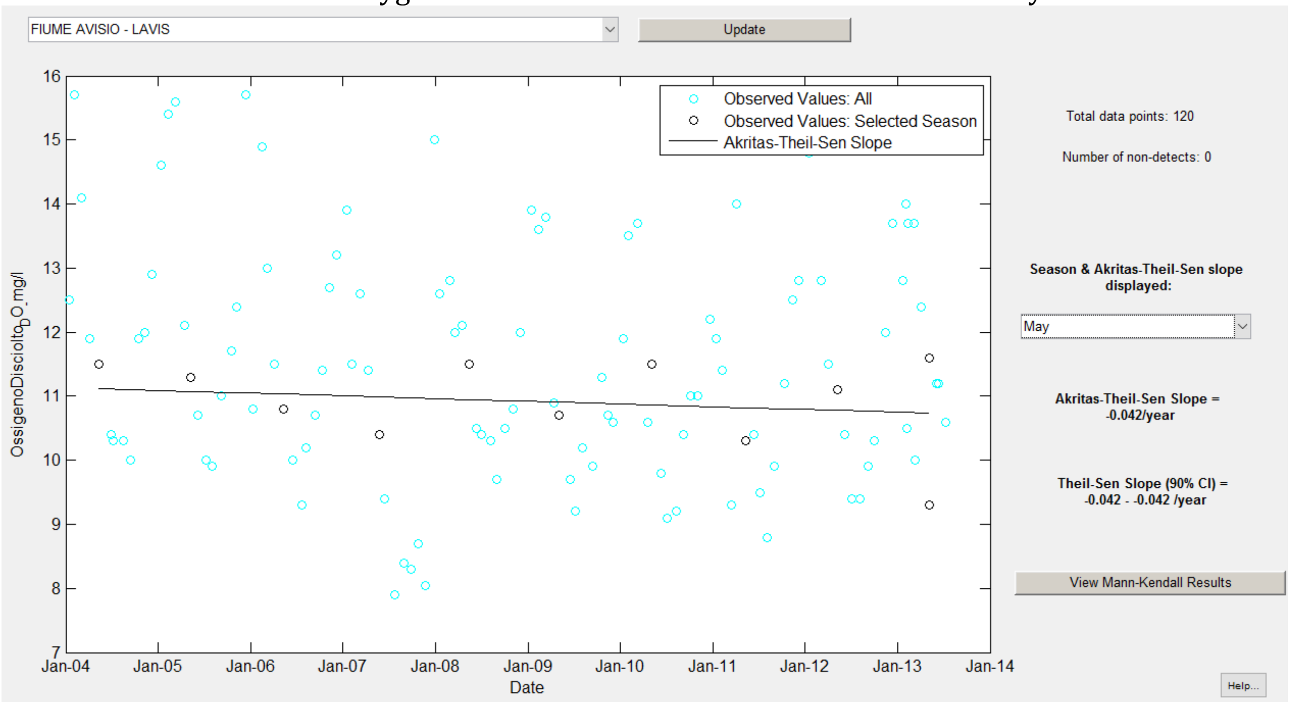


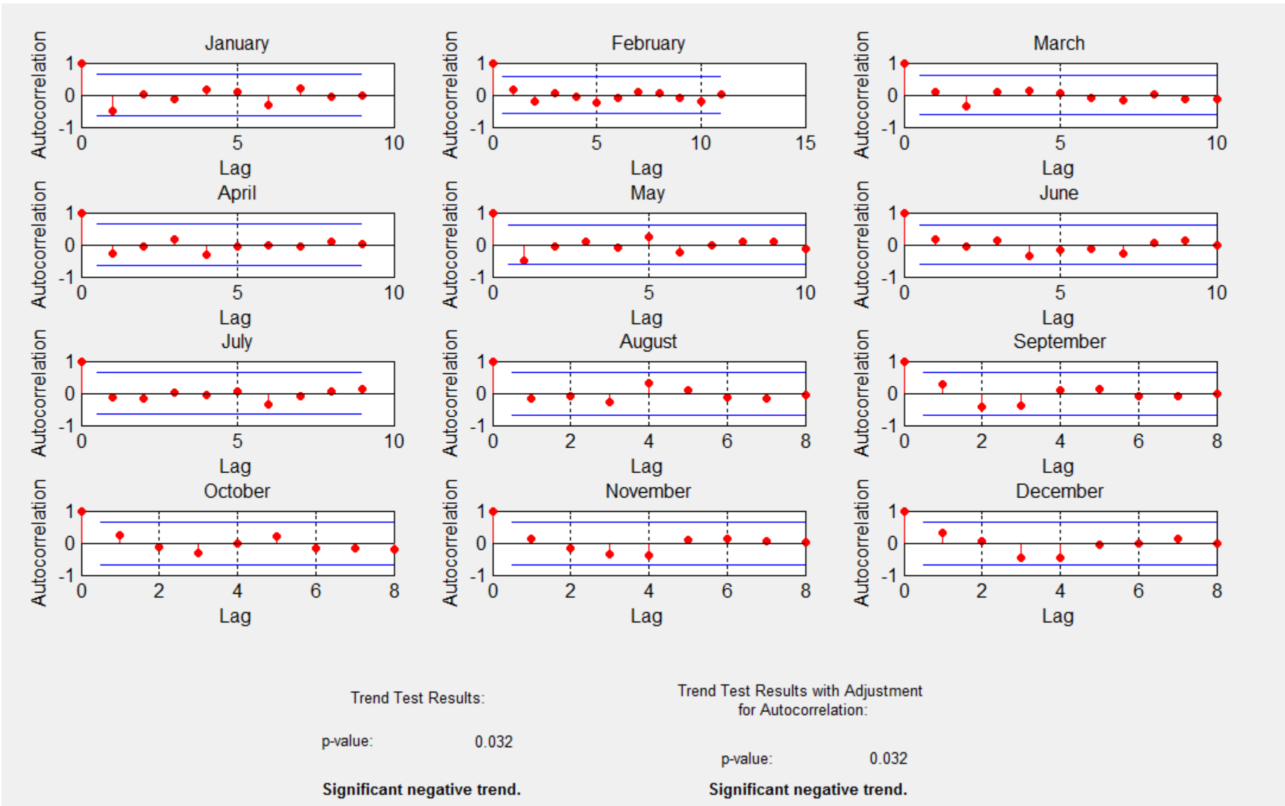




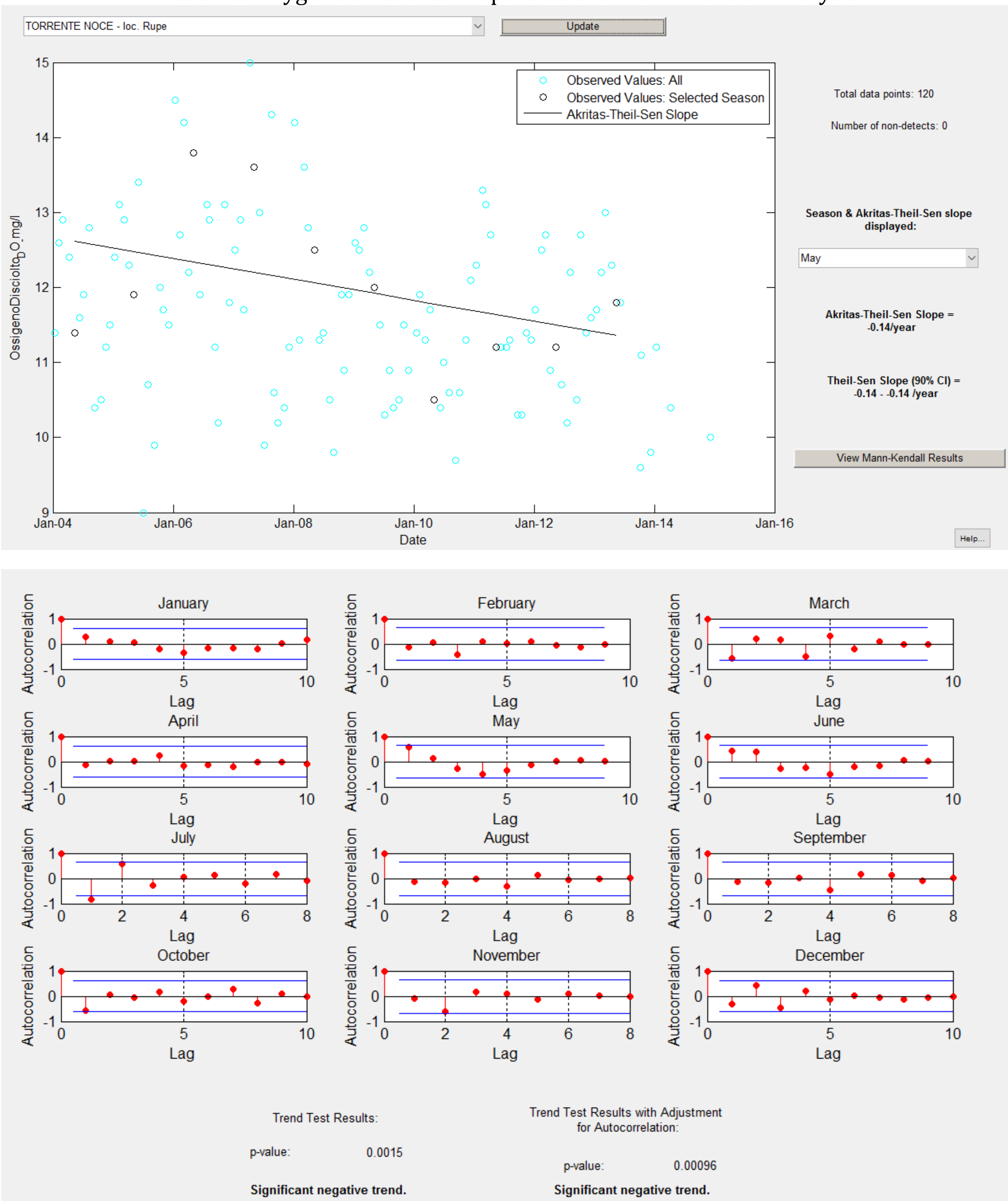


Dissolved Oxygen at Avisio-Lavis: Seasonal Mann-Kendall Analysis

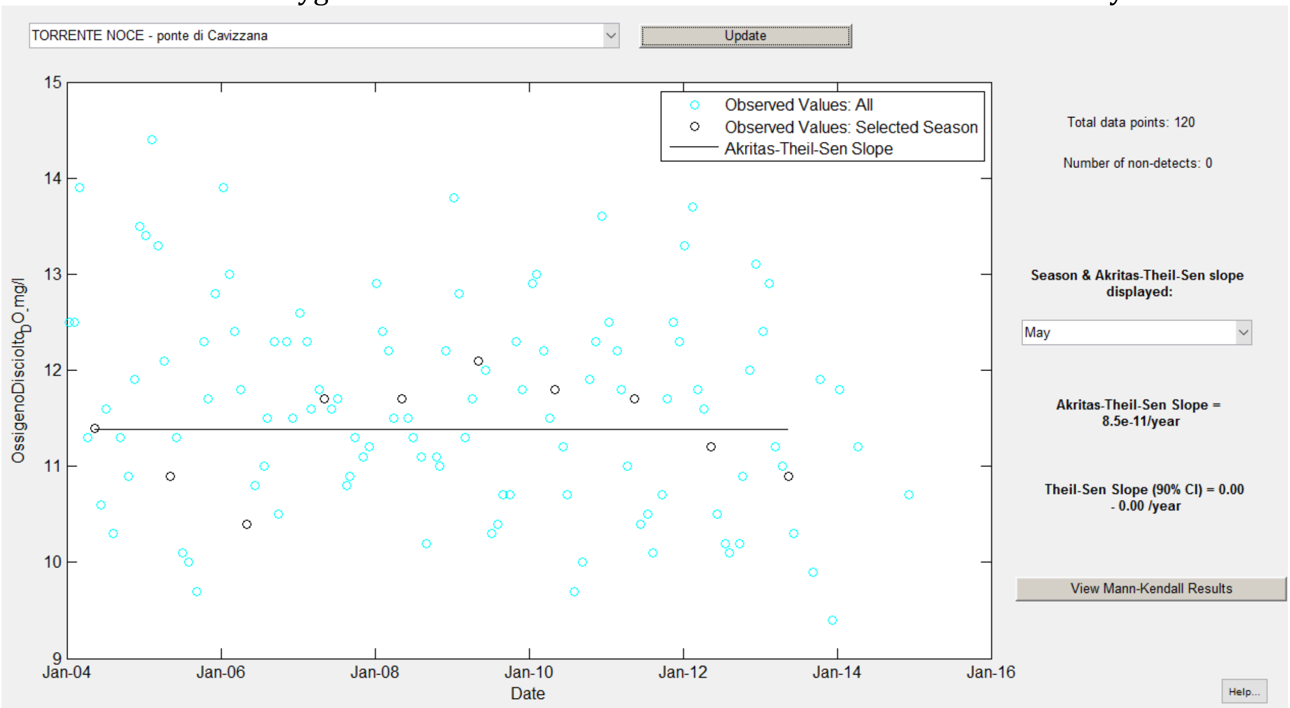


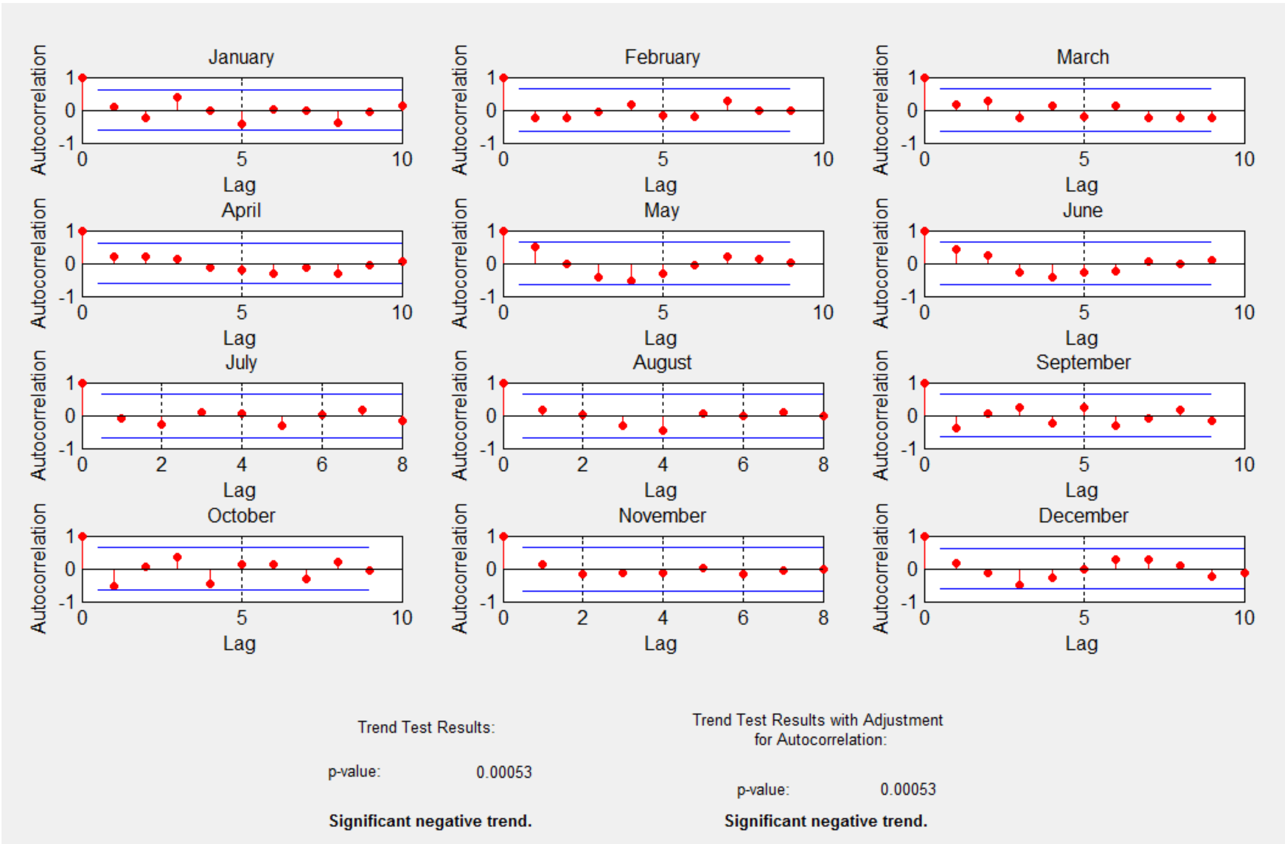


Dissolved Oxygen at Noce-loc. Rupe: Seasonal Mann-Kendall Analysis



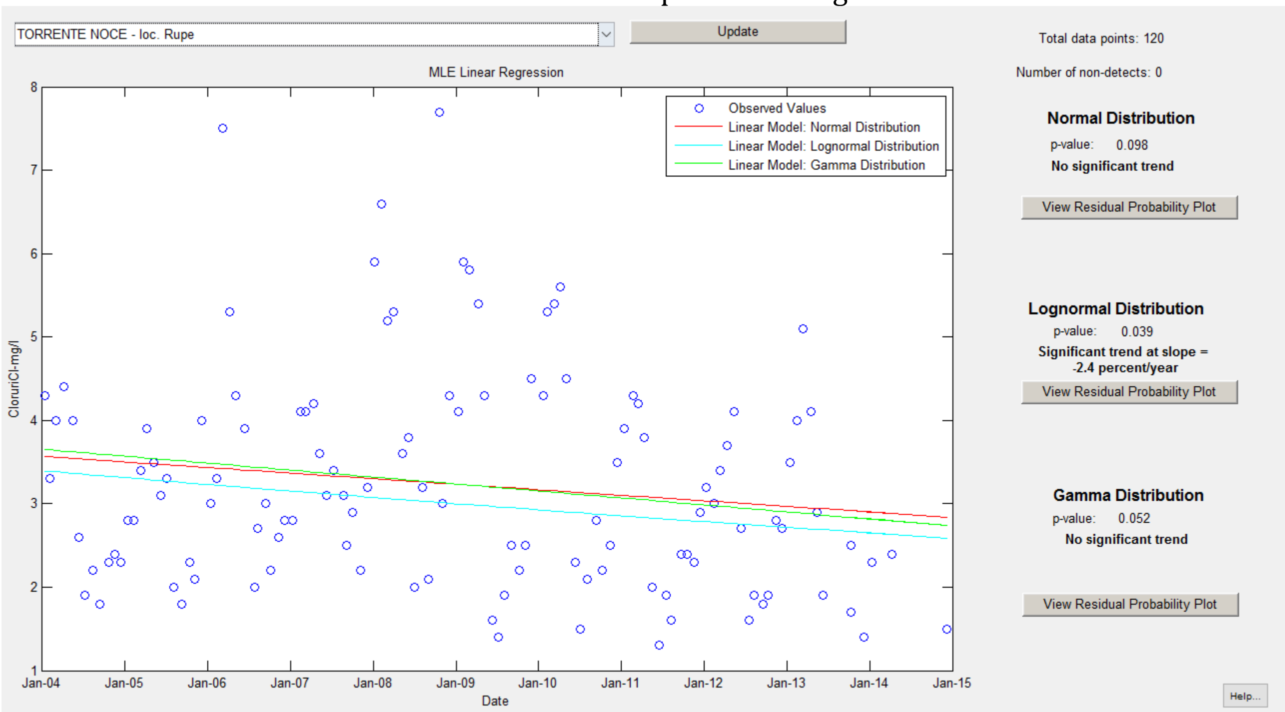
Dissolved Oxygen at Noce-Ponte di Cavizzana: Seasonal Mann-Kendall Analysis

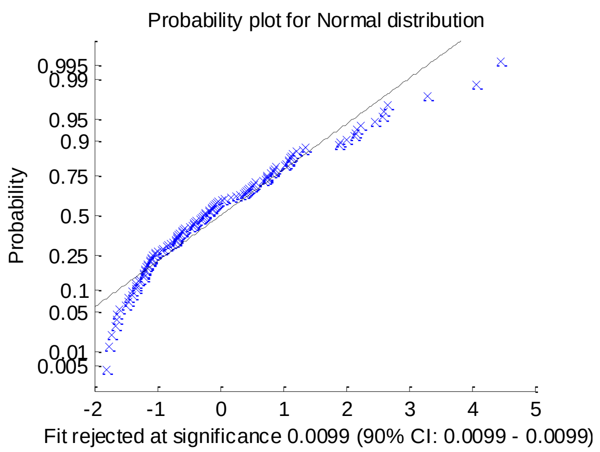


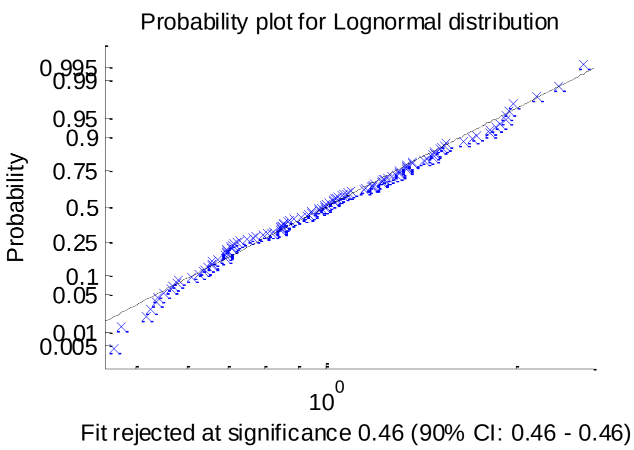


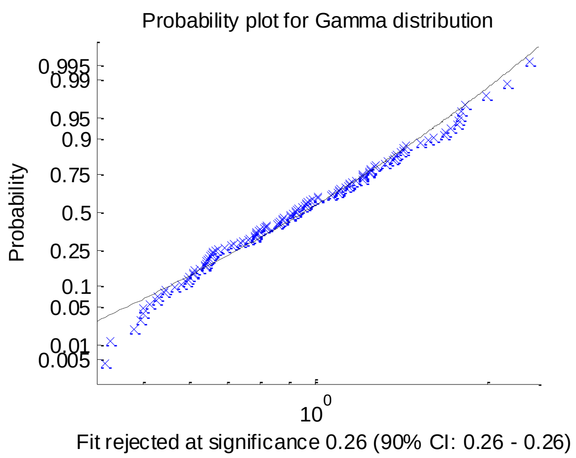
Appendix C-3: Adige Catchment Trend Analysis Case Study Results – Chloride

Chloride at Noce-loc. Rupe: Linear Regression

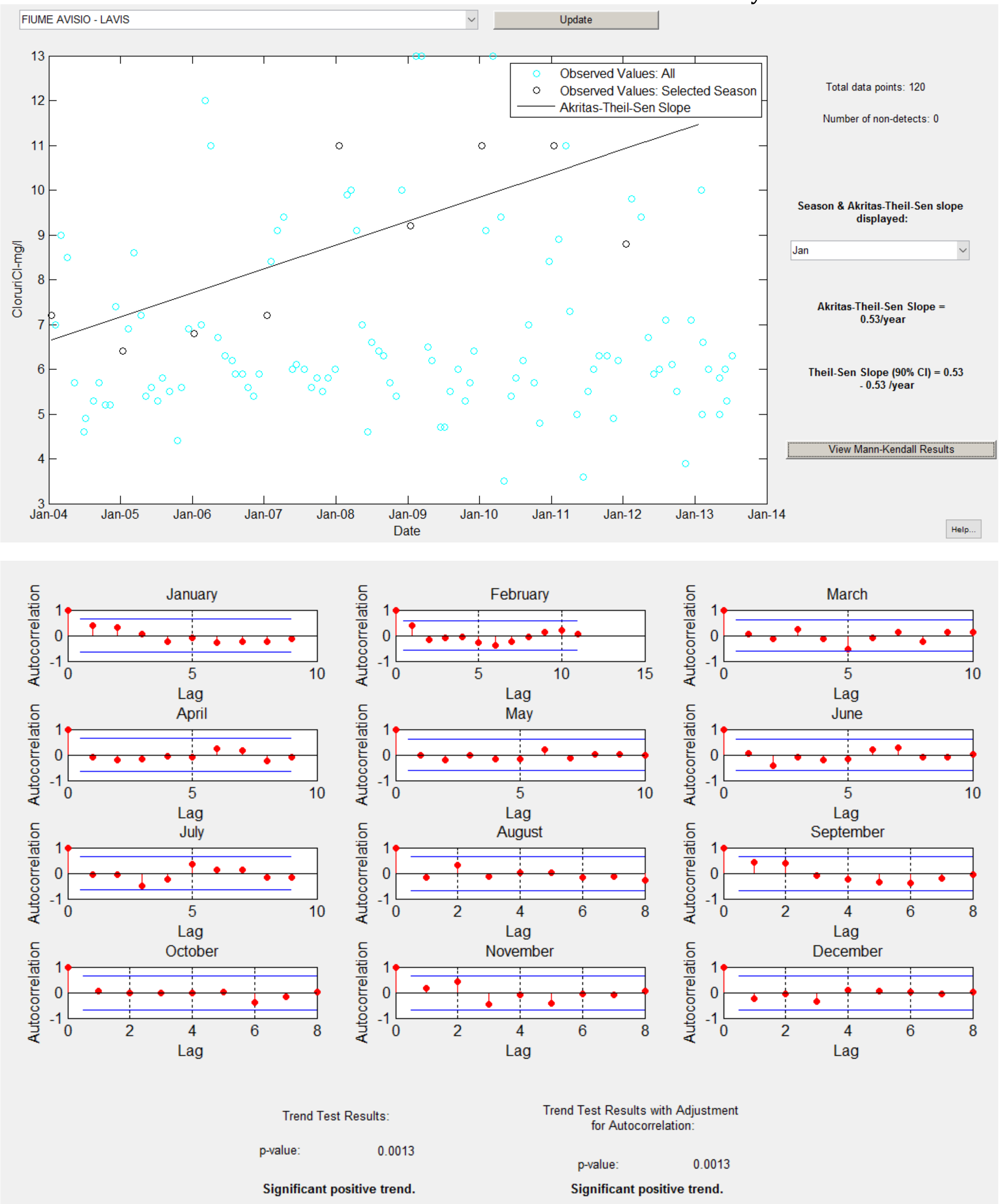




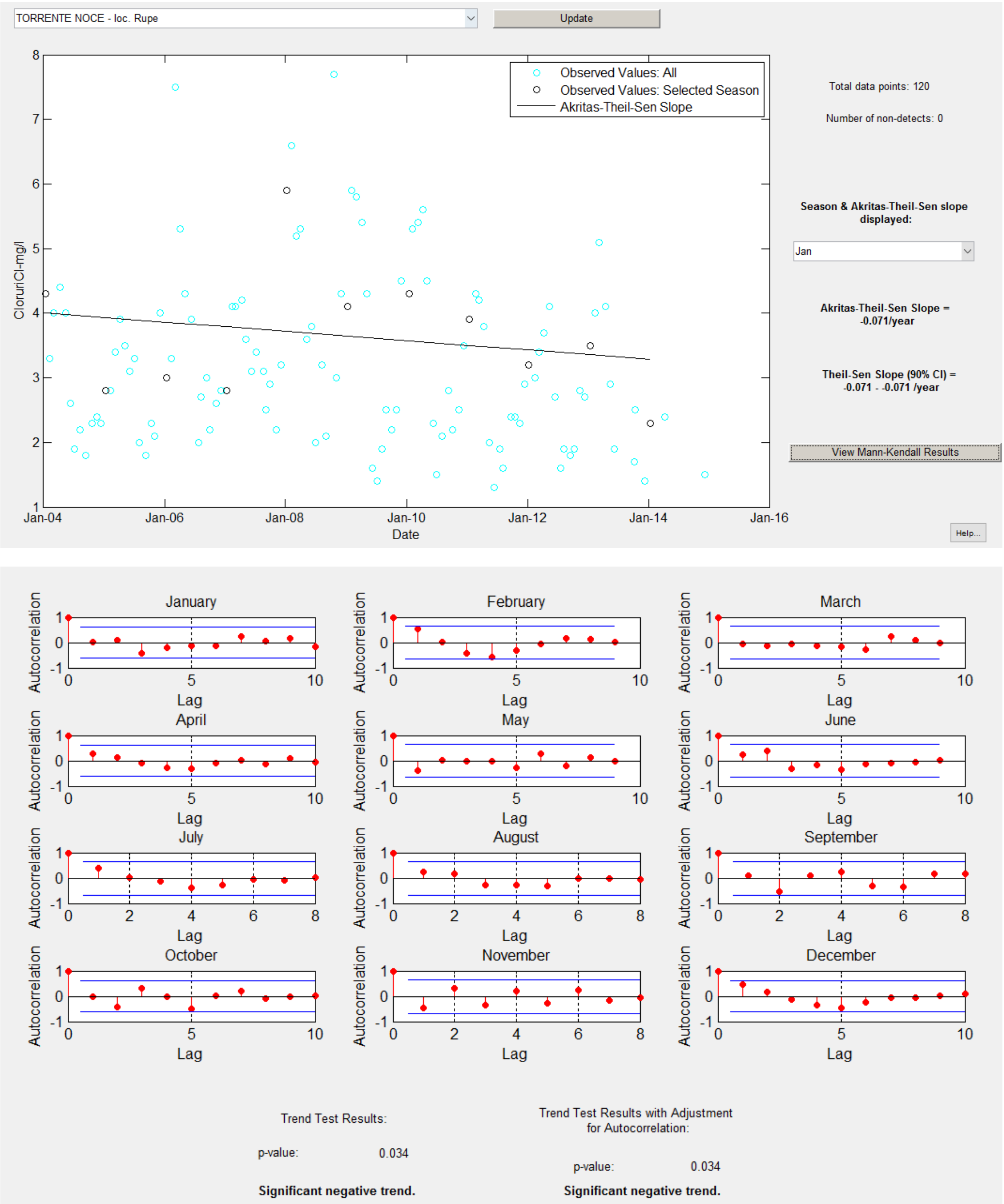




Chloride at Avisio-Lavis: Seasonal Mann-Kendall Analysis

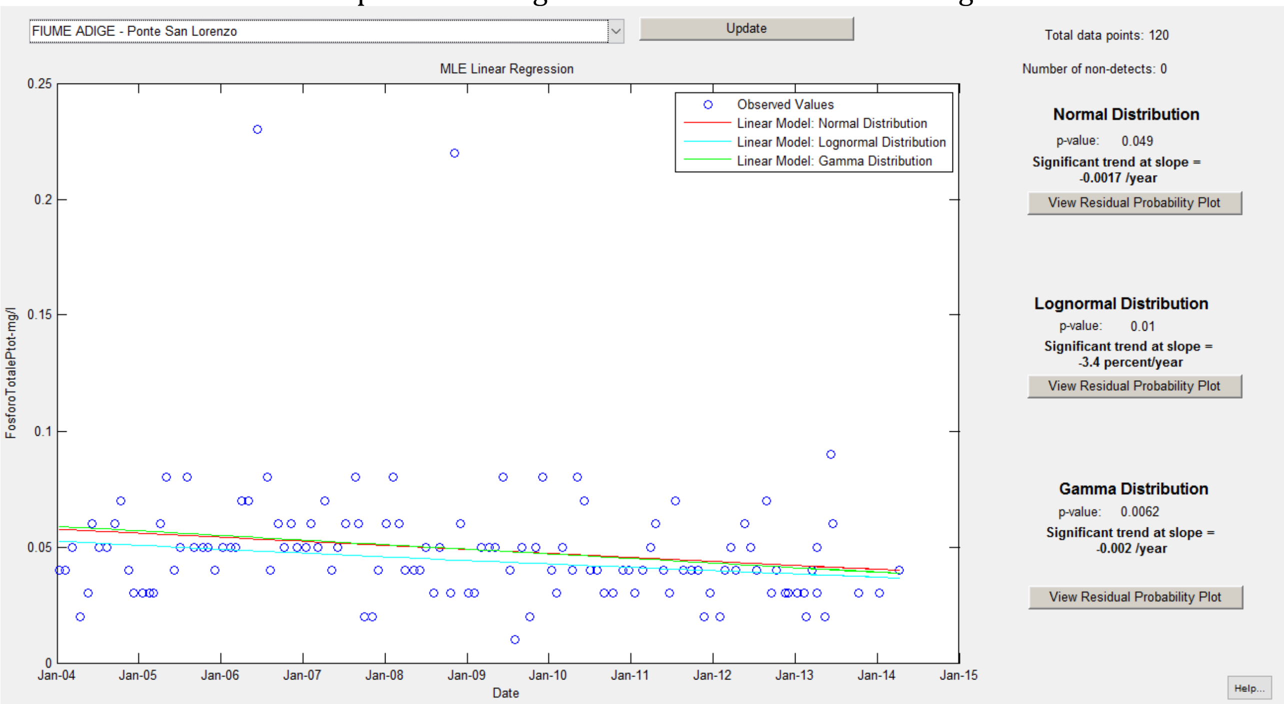


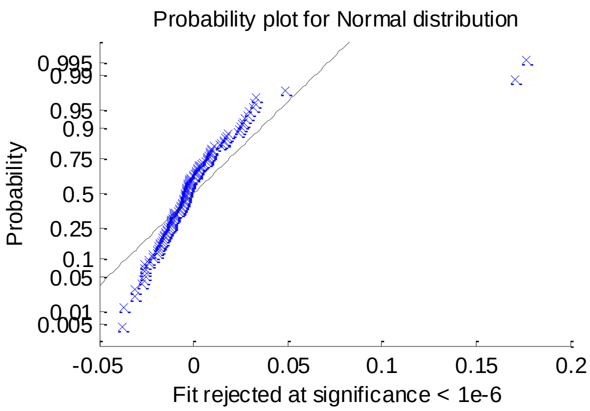
Chloride at Noce-loc. Rupe: Seasonal Mann-Kendall Analysis

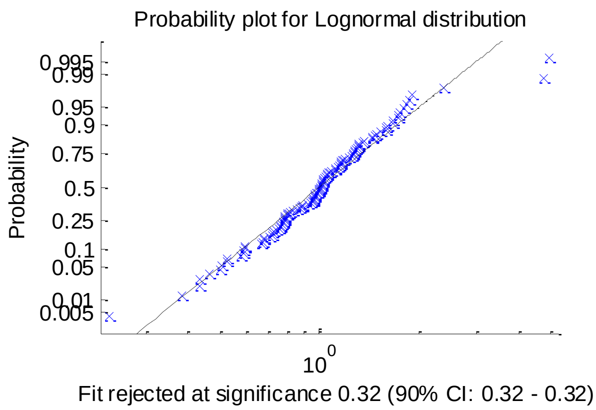


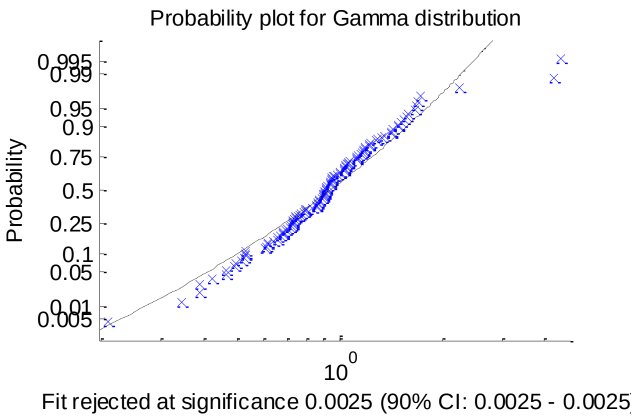
Appendix C-4: Adige Catchment Trend Analysis Case Study Results – Total Phosphorus

Total Phosphorus at Adige-Ponte San Lorenzo: Linear Regression

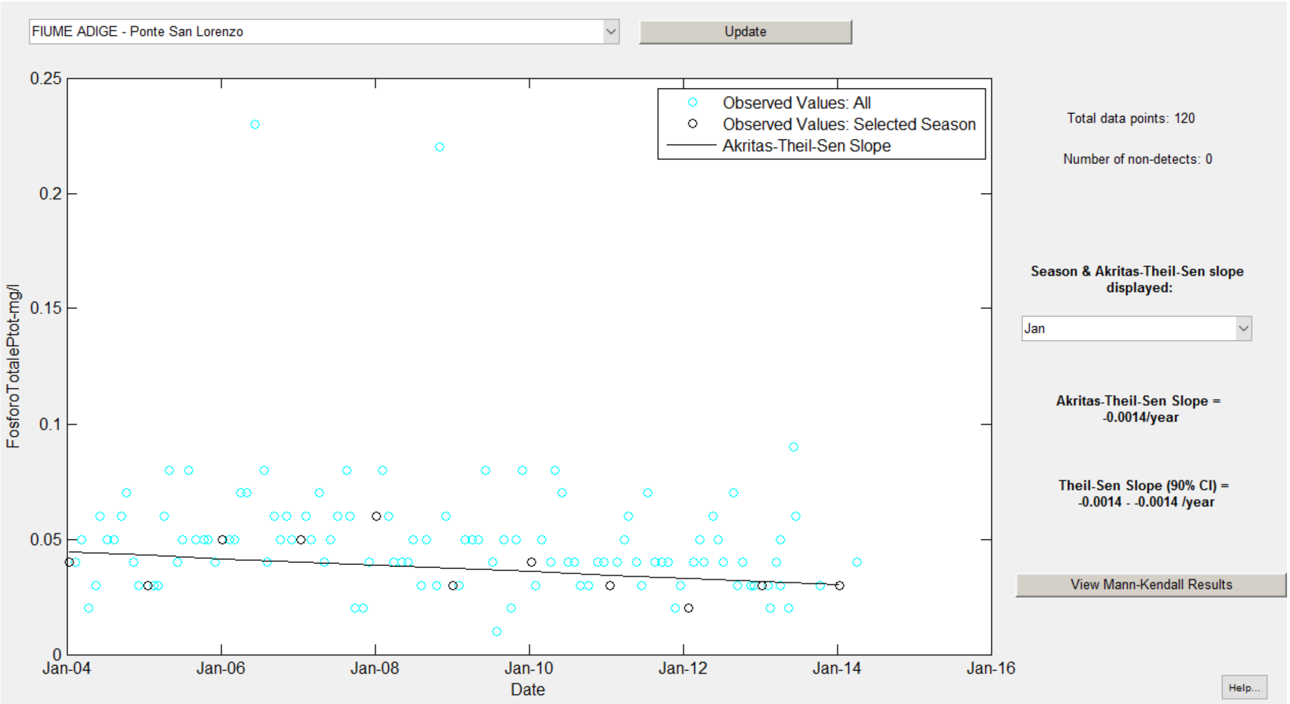


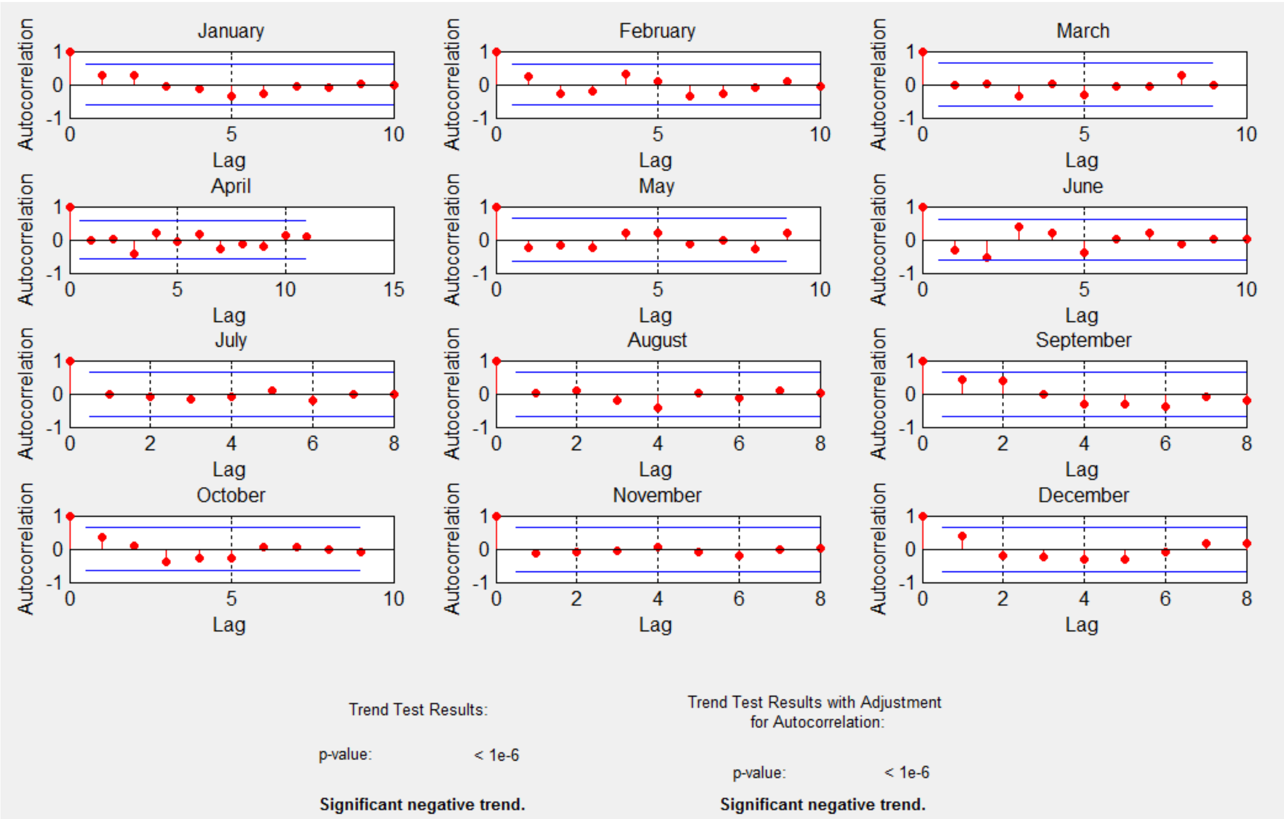




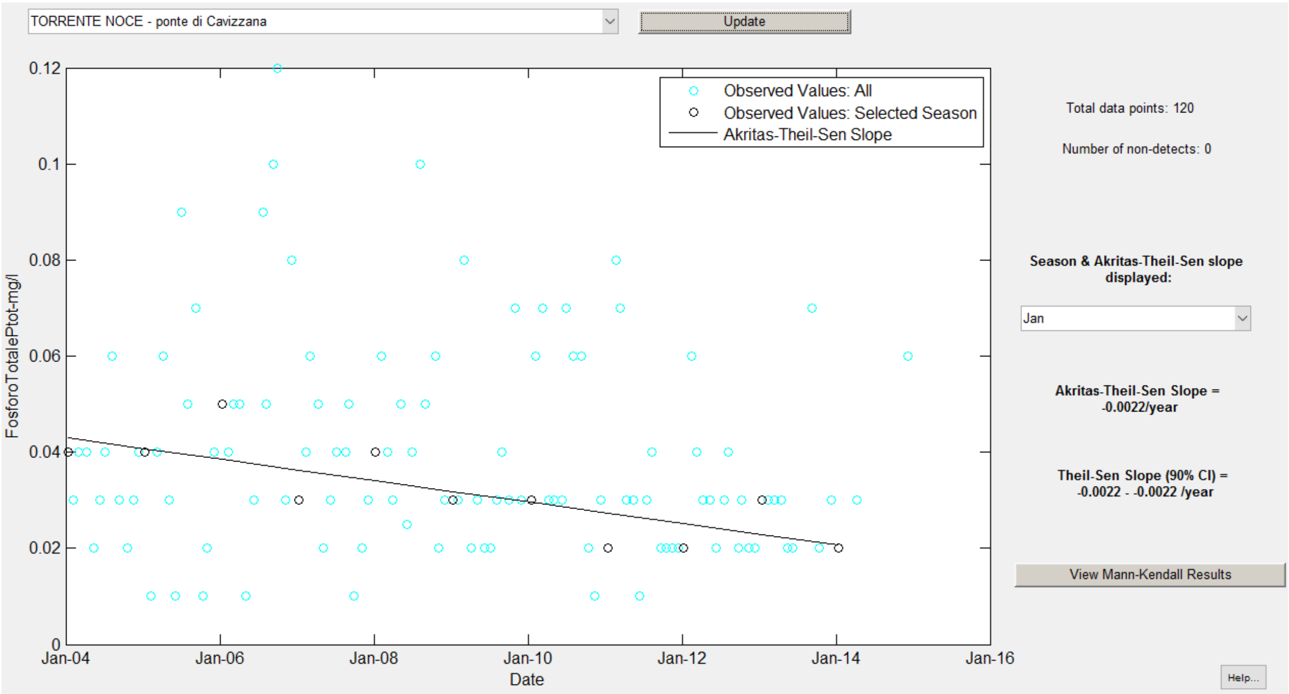


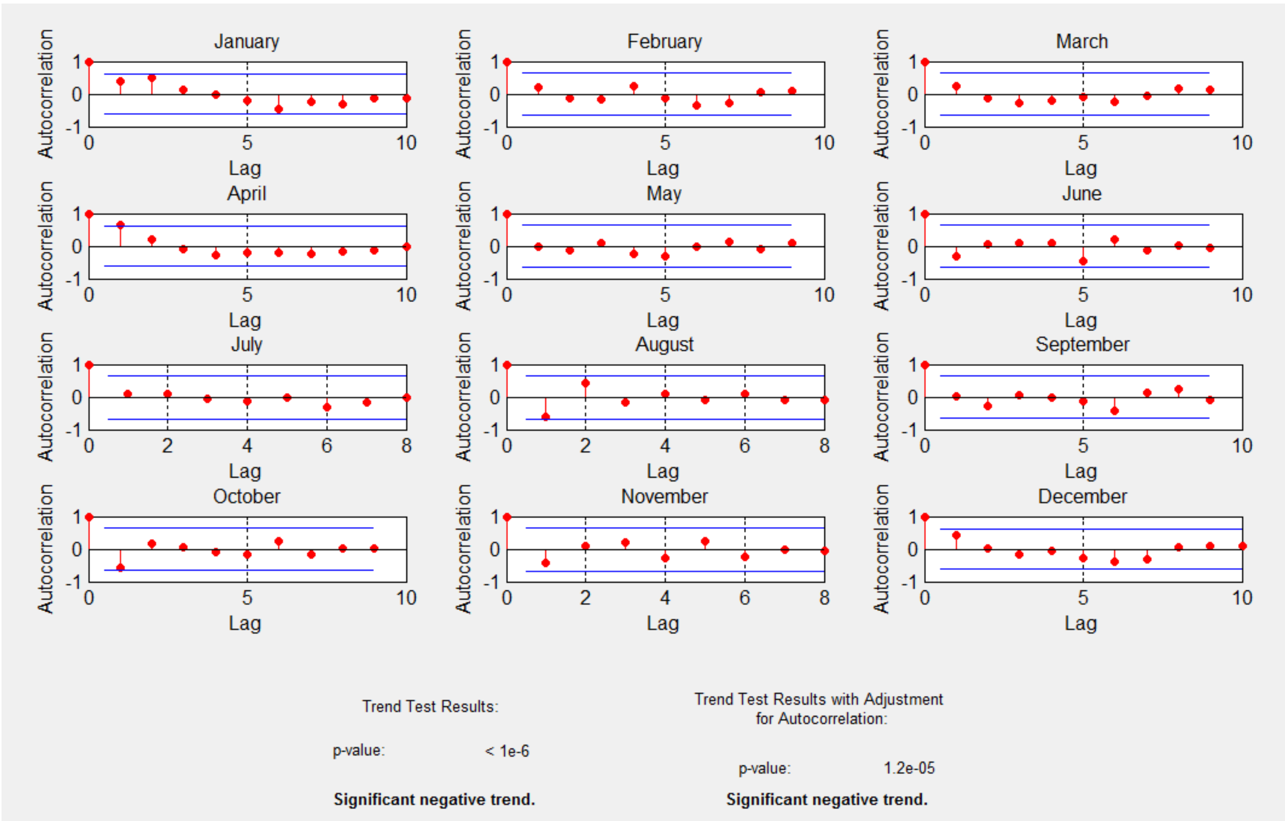
Total Phosphorus at Adige-Ponte San Lorenzo: Seasonal Mann-Kendall Analysis





Total Phosphorus at Noce-Ponte di Cavizzana: Seasonal Mann-Kendall Analysis





Appendix C-5: Adige Catchment Trend Analysis Case Study Results – Conductivity

Conductivity at Adige-Ponte San Lorenzo: Seasonal Mann-Kendall Analysis