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User guide to Exploration and Graphics for RivEr Trends (EGRET) and dataRetrieval: R packages for hydrologic data

By Robert M. Hirsch and Laura De Cicco

Techniques and Methods

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Contents

Figures vi

Tables ix

Conversion Factors xi

Abstract 1

Introduction 2

Organization of this report 4

Getting help with functions 5

Package Installation 7

Data Entry 7

Overview of data entry 7

Mean daily discharge data for use in EGRET 8

Discharge data from USGS data service 10

Discharge data from a text file 13

Water quality data for use in EGRET 15

Water Quality Data from USGS Web Services 18

Water Quality Data from EPA STORET Data Service 20

Water Quality Data from a User Supplied File 20

Entry and storage of meta-data 21

Moving discharge data from the Daily data frame to the Sample data frame 25

Removing duplicate observations 25

Saving the workspace for future use 26

Setting the period of analysis for graphs, tables, and analyses in EGRET 27

Selection of units of measurement for graphs and tables in EGRET 29

Flow History Analysis 31
Introduction 31
The smoothing method used in flow history analyses 33
EGRET functions for flow history analysis 36
The function `setPA` 37
The function `makeAnnualSeries` 37
Plotting the results for a single discharge statistic using `plotFlowSingle` 39
Printing out results for a single discharge statistic using `printSeries` and `tableFlowChange` 40
Plot changes in variability with `plotSDLogQ` 43
Graphics for plotting the discharge record, `plotQTimeDaily` 46
Multipanel graphics for flow history 48
Summarizing Water Quality Data (without using WRTDS) 53
plotConcTime 55
flowDuration 62
plotConcQ 63
plotFluxQ 67
boxConcMonth 68
boxQTwice 70
multiPlotDataOverview 71
WRTDS analysis of water quality data 73
Overview 73
Estimates of concentration and flux 74
Estimation of flow-normalized concentration and flux 81
Fitting the WRTDS model 85

Displaying and managing WRTDS model results 90
Computing monthly results 90
Issues of large data gaps - using the `blankTime` function 91
Plotting annual results 92
Producing tables of results 97
Computing and displaying tables of change over time 98
Exploring the quality of the fitted model - overview 102
Flux bias statistic 104
Graphics for examining the quality of the model 106
Exploring model behavior and adjusting model parameters 122
plotContours 122
Introducing an example case: Maumee River, Ohio, Dissolved Reactive Phosphorus 129
plotConcQSmooth 134
plotConcTimeSmooth 147
Editing data sets 151
Deleting values 153
Shortening the Period of Record 153
Create interval concentrations 153
Working with multiple versions of data frames 155
Batch processing in EGRET 159
References Cited 161

Figures

Figure 1: Example of the output from the mergeReport function. 25

Figure 2. Computer input and output showing the available choices of discharge units and flux units. 30

Figure 3: Values of the triCube weight function used in weighted regressions for smoothing discharge time series. Half-width is set to its default value of 30 years. 36

Figure 4. Plot of the 7-day minimum discharge by year (dots) and smoothed estimates (curve). 40

Figure 5. Output of the annual 7-day minimum discharge and smoothed values of annual 7-day minimum discharge in mm/day. 41

Figure 6. Example output from `tableFlowChange`. ..... **Error! Bookmark not defined.**

Figure 7. Graph of the standard deviation of Log(Q) over time, Colorado River at Lees Ferry, AZ. 45

Figure 8. Graph of daily discharge record for the Big Sioux RIver at Akron, IA 46

Figure 9. Output from `plotQTimeDaily` for Discharge data for Big Sioux River at Akron Iowa, showing discharges only above 600 m^3/s. 47

Figure 10. Example of graphics produced by `plotFour` function. 49

Figure 11. Output from `plotFour` for the Merced River. 50

Figure 12. Output from `plot15`, Merced River at Happy Isles Bridge near Yosemite, CA. 53

Figure 13. Concentration versus time, Choptank River near Greensboro Maryland, Nitrate. 56

Figure 14. Concentration versus time, Choptank River near Greensboro, Maryland, Nitrate, for April, May and June 57

Figure 15. Choptank River near Greensboro, MD, Nitrate, for April, May, June, discharge between 34 and 165 ft^3/s. 59

Figure 16. Choptank River near Greensboro, MD, Nitrate concentration for months of April - June, for discharge greater than 165 ft^3/s. 61

Figure 17. Output from flowDuration function. 62

Figure 18. Output from flowDuration function, with span = 45 days and center date is May 16.....63
Figure 19. Concentration versus discharge, Choptank River near Greensboro Maryland, Nitrate.....64
Figure 20. Concentration versus discharge, with concentration on a log scale, for the Choptank River near Greensboro Maryland.....66
Figure 21. Flux versus discharge plot, Choptank River near Greensboro, MD.....68
Figure 22. Boxplots by month for the Iowa River at Wapello, IA for nitrate.....69
Figure 23. Output from the function boxQTwice for Choptank River near Greensboro, MD.....71
Figure 24. Output from multPlotDataOverview function for nitrate data from the Iowa RIver at Wapello, IA.....72
Figure 25. Contour plot of expected value of chloride concentration as a function of time and discharge, Milwaukee River at Milwaukee, WI.....75
Figure 26. Contour plots of fitted WRTDS model for Milwaukee River Chloride data, showing the years 2000-2003. Upper panel is the estimate of the ln(*c*) surface, middle panel is the estimate of the standard error and bottom panel is the estimate of concentration.....78
Figure 27. Observed and estimated concentrations (upper panel), observed and estimated fluxes (lower panel). Chloride, Milwaukee River. In each panel, the dots represent the observations and the line represents to WRTDS estimates for all of the days.....81
Figure 28. Concentration history graphic produced by plotConcHist function. Choptank River, MD, nitrate data.....95
Figure 29. Flux history graphic produced by plotFluxHist function. Choptank River, MD, nitrate data.....96
Figure 30. Example output from `tableResults`, for Potomac River at Washington, DC, Atrazine data.....98
Figure 31. Output from `tableChange` function for Potomac River at Washington DC, Atrazine.....100
Figure 32. Output of fluxBiasMulti function for Nitrate for the Vermilion River at Pontiac, IL. Description of each of the 8 panels is presented in the text of the report.....109
Figure 33. Output of fluxBiasMulti function for Nitrate, Vermilion River at Pontiac, IL using a model approximating LOADEST 5.....110

Figure 34. Output of plotConcTimeDaily for the years 1992-1994, for the WRTDS model of nitrate for the Vermilion River at Pontiac, IL. 119
Figure 35. Output of plotConcTimeDaily for the years 1992-1994, for the model that approximates the LOADEST 5 model, for the Vermilion River at Pontiac, IL. 121
Figure 36. Contour plot for nitrate, Vermillion River at Pontiac, IL. Year designations on the horizontal axis indicate the start of the calendar year. 126
Figure 37. Contour plot of the estimated standard error of log(concentration) using the WRTDS model. 128
Figure 38. Contour plot of Dissolved Reactive Phosphorus, Maumee River at Waterville, OH, For three, two-year time periods. 131
Figure 39. Difference contours for Dissolved Reactive Phosphorus, Maumee River at Waterville, OH, comparing 1988 to 2011 133
Table 11. Arguments for the function `plotConcQSmooth`. 134
Figure 40. Concentration versus discharge relationship centered on August 1 for three different years, for dissolved reactive phosphorus, Maumee River at Waterville, Ohio. 137
Figure 41. Concentration versus discharge relationship centered on May 1 for three different years, for dissolved reactive phosphorus, Maumee River at Waterville, Ohio. 139
Figure 42. Concentration versus discharge relationship centered on three dates (January 1, May 1, and September 1) of 2010, for dissolved reactive phosphorus, Maumee River at Waterville, Ohio. 141
Figure 43 Concentration versus discharge relationship centered on three dates (January 1, May 1, and September 1) of 2010, with the discharge smoothing parmeter (windowQ = 1 rather than windowQ = 2) for dissolved reactive phosphorus, Maumee River at Waterville, Ohio. 143
Figure 44. Concentration versus discharge relationship centered on three dates (April 1, August 1, and December 1) of 2010, for dissolved reactive phosphorus, Maumee River at Waterville, Ohio, but shown with a discharge scale extended to excessively low values. 145

Figure 45. Concentration versus time plots for 3 different discharge values, for dissolved reactive phosphorus, Maumee River at Waterville, Ohio, centered on September 1 of each year 150

Tables

Table 1. A list of the column names for the `Daily` data frame. Those shown in black are computed from the date and discharge information retrieved and stored when the data frame is created. Those in red are created and stored automatically when the WRTDS computations are made by the EGRET package using the `modelEstimation` function. 9

Table 2. A list of column names for the Sample data frame. Those shown in black are computed and stored when the data freame is created. Those in red are created and stored automatically when the WRTDS computations are made by the EGRET package using the `modelEstimation` function. 15

Table 3. Variables required in the INFO data frame for use in EGRET applications. 22

Table 4. Examples of the Period of Analysis and the paStart and paLong values associated with them. 28

Table 5. Definitions of the eight discharge statistics computed in EGRET 38

Table 6. Important arguments for the function `plotConcTime` 55

Table 7. Information about the 5 arguments used in modelEstimation. 85

Table 8. Column names for the data frame `AnnualResults`. 89

Table 9. Commonly used arguments for `plotConcHist`. 93

Table 10. Arguments to the `plotContours` function. 124

Table 12. Arguments for the function `plotConcTimeSmooth` 148

Conversion Factors

Inch/Pound to SI

Multiply	By	To obtain
	Area	
square mile (mi^2)	2.590	square kilometer (km^2)
	Volume	
million gallons (Mgal)	3,785	cubic meter (m^3)
cubic foot (ft^3)	28.32	cubic decimeter (dm^3)
cubic foot (ft^3)	0.02832	cubic meter (m^3)
acre-foot (acre-ft)	1,233	cubic meter (m^3)
acre-foot (acre-ft)	0.001233	cubic hectometer (hm^3)
	Flow rate	
acre-foot per day (acre-ft/d)	0.01427	cubic meter per second (m^3/s)
acre-foot per year (acre-ft/yr)	1,233	cubic meter per year (m^3/yr)
acre-foot per year (acre-ft/yr)	0.001233	cubic hectometer per year (hm^3/yr)
cubic foot per second (ft^3/s)	0.02832	cubic meter per second (m^3/s)
cubic foot per second per square mile [$(ft^3/s)/mi^2$]	0.01093	cubic meter per second per square kilometer [$(m^3/s)/km^2$]
cubic foot per day (ft^3/d)	0.02832	cubic meter per day (m^3/d)
gallon per day (gal/d)	0.003785	cubic meter per day (m^3/d)
gallon per day per square mile [$(gal/d)/mi^2$]	0.001461	cubic meter per day per square kilometer [$(m^3/d)/km^2$]
million gallons per day (Mgal/d)	0.04381	cubic meter per second (m^3/s)
million gallons per day per square mile [$(Mgal/d)/mi^2$]	1,461	cubic meter per day per square kilometer [$(m^3/d)/km^2$]
inch per hour (in/h)	0 .0254	meter per hour (m/h)
inch per year (in/yr)	25.4	millimeter per year (mm/yr)
	Mass	
ounce, avoirdupois (oz)	28.35	gram (g)
pound, avoirdupois (lb)	0.4536	kilogram (kg)
ton, short (2,000 lb)	0.9072	megagram (Mg)
ton, long (2,240 lb)	1.016	megagram (Mg)
ton per day (ton/d)	0.9072	metric ton per day
ton per day (ton/d)	0.9072	megagram per day (Mg/d)
ton per day per square mile [$(ton/d)/mi^2$]	0.3503	megagram per day per square kilometer [$(Mg/d)/km^2$]
ton per year (ton/yr)	0.9072	megagram per year (Mg/yr)

ton per year (ton/yr)	0.9072	metric ton per year

Temperature in degrees Celsius (°C) may be converted to degrees Fahrenheit (°F) as follows:

°F=(1.8×°C)+32

Temperature in degrees Fahrenheit (°F) may be converted to degrees Celsius (°C) as follows:

°C=(°F-32)/1.8

Vertical coordinate information is referenced to the insert datum name (and abbreviation) here for instance, “North American Vertical Datum of 1988 (NAVD 88).”

Horizontal coordinate information is referenced to the insert datum name (and abbreviation) here for instance, “North American Datum of 1983 (NAD 83).”

Altitude, as used in this report, refers to distance above the vertical datum.

SI to Inch/Pound

Multiply	By	To obtain
	Length	
millimeter (mm)	0.03937	inch (in.)
meter (m)	3.281	foot (ft)
kilometer (km)	0.6214	mile (mi)
	Area	
square kilometer (km^2)	0.3861	square mile (mi^2)
	Volume	
liter (L)	33.82	ounce, fluid (fl. oz)
liter (L)	2.113	pint (pt)
liter (L)	1.057	quart (qt)
liter (L)	0.2642	gallon (gal)
cubic meter (m^3)	264.2	gallon (gal)
cubic meter (m^3)	0.0002642	million gallons (Mgal)
cubic meter (m^3)	35.31	cubic foot (ft^3)
cubic meter (m^3)	1.308	cubic yard (yd^3)
cubic meter (m^3)	0.0008107	acre-foot (acre-ft)
	Flow rate	
cubic meter per second (m^3/s)	70.07	acre-foot per day (acre-ft/d)
cubic meter per second (m^3/s)	35.31	cubic foot per second (ft^3/s)
cubic meter per second per square kilometer [$(m^3/s)/km^2$]	91.49	cubic foot per second per square mile [$(ft^3/s)/mi^2$]
cubic meter per day (m^3/d)	35.31	cubic foot per day (ft^3/d)
cubic meter per day per square kilometer [$(m^3/d)/km^2$]	684.28	gallon per day per square mile [$(gal/d)/mi^2$]
cubic meter per second (m^3/s)	22.83	million gallons per day (Mgal/d)
cubic meter per day per square kilometer [$(m^3/d)/km^2$]	0.0006844	million gallons per day per square mile [$(Mgal/d)/mi^2$]
millimeter per year (mm/yr)	0.03937	inch per year (in/yr)
	Mass	
gram (g)	0.03527	ounce, avoirdupois (oz)
kilogram (kg)	2.205	pound avoirdupois (lb)
megagram (Mg)	1.102	ton, short (2,000 lb)
megagram (Mg)	0.9842	ton, long (2,240 lb)
metric ton per day	1.102	ton per day (ton/d)
megagram per day (Mg/d)	1.102	ton per day (ton/d)
megagram per day per square kilometer [$(Mg/d)/km^2$]	2.8547	ton per day per square mile [$(ton/d)/mi^2$]

megagram per year (Mg/yr)	1.102	ton per year (ton/yr)
metric ton per year	1.102	ton per year (ton/yr)

Temperature in degrees Celsius (°C) may be converted to degrees Fahrenheit (°F) as follows:

°F=(1.8×°C)+32

Temperature in degrees Fahrenheit (°F) may be converted to degrees Celsius (°C) as follows:

°C=(°F-32)/1.8

Vertical coordinate information is referenced to the insert datum name (and abbreviation) here, for instance, “North American Vertical Datum of 1988 (NAVD 88)”

Horizontal coordinate information is referenced to the insert datum name (and abbreviation) here, for instance, “North American Datum of 1983 (NAD 83)”

Altitude, as used in this report, refers to distance above the vertical datum.

User guide to Exploration and Graphics for RivEr Trends (EGRET) and dataRetrieval: R packages for hydrologic data

By Robert M. Hirsch and Laura De Cicco

Abstract

Evaluating long-term changes in river conditions (water quality and discharge) is an important use of hydrologic data. To carry out such evaluations the hydrologist needs tools to facilitate several key steps in the process: acquiring the data records from a variety of sources, structuring it in ways that facilitate the analysis, routines that will process the data to extract information about changes that may be happening, and graphical techniques that can display findings about change. A pair of tightly-linked R packages, called dataRetrieval and EGRET (Exploration and Graphics for RivEr Trends) have been developed for carrying out each of these steps in an integrated manner. They are designed to easily accept data from three sources: U.S. Geological Survey hydrologic data, EPA STORET data, and user-supplied flat files. The dataRetrieval package not only serves as a "front end" to the EGRET package but can also be used to easily download many types of hydrologic data and organize it ways that facilitate many other hydrologic applications. The EGRET package has components oriented towards the description of long-term changes in streamflow statistics (high flow, average flow and low flow) as well as changes in water quality. For the water quality analysis it uses Weighted Regressions on Time,

Discharge and Season (WRTDS) to describe long-term trends in both concentration and flux. EGRET also creates a wide range of graphical presentations of the water quality data and of the WRTDS results. This report serves as a user guide to these two R packages, providing detailed guidance on installation and use of the software, documentation of the analysis methods used, as well as guidance on some of the kinds of questions and approaches that the software can facilitate.

Introduction

The analysis of data about rivers, their flow and their quality, depends on having a set of tools that are appropriate to the nature of the data and to the questions that one wishes to answer. An important component of the analysis tool is having a straight-forward method of obtaining the data, checking it, and structuring it in a way that facilitates the analysis. This report is a guide to a tightly coupled system of software for doing both the data retrieval and the data analysis. This system is made up of two R-packages (R Core Team, 2013); R is a free software environment for statistical computing and graphics. It compiles and runs on a wide variety of UNIX platforms, Windows, and MacOS.

The first of these packages is known as dataRetrieval. It is designed to obtain water quality sample data, daily, instantaneous, and metadata directly from the USGS NWIS (National Water Information System) data services (Geological Survey (U.S.), 1998) as well as water quality data from the Water Quality Portal (Scott and others, 2008). It also allows for user-supplied text files as inputs for each of these data types. The program is designed to ingest the data directly into R and organize them into file structures suited to the analysis.

The second of these packages is known as EGRET, which stands for Exploration and Graphics for RivEr Trends. The underlying objective of EGRET is to enable the hydrologist to explore various types of river data and describe, quantify, and visualize the behavior of these variables: discharge, concentrations of an analyte (such as a major ion, a nutrient, or suspended sediment), and fluxes of an

analyte. It can describe long-term averages, the patterns of variability, as well as temporal trends in these variables. The focus of EGRET can best be described under the general heading of exploratory data analysis (Tukey, 1977) as opposed to statistical inference or hypothesis testing. Within that overall framework EGRET carries out three types of tasks.

1. The first is referred to as the flow history component of EGRET. It provides a variety of tabular and graphical outputs focused on discharge statistics such as the annual mean, annual 7-day low flow, annual 1-day maximum, as well as seasonal or monthly versions of these. All of these are based on time-series smoothing methods. It was designed for studies of long-term discharge change that may be focused on questions such as how discharge may be changing as a result of changes in climate, land use, water use, or water management. It works best for complete daily discharge data sets of 50 years or longer.
2. The second is the graphical display of water quality sample data as they vary in relationship to time, discharge, or season. All of the EGRET functionality for water quality assumes that there is a complete record of daily discharge data for the site at which the water quality data were collected (or sufficiently close to the site so that it provides a good representation of discharge conditions at the site). This discharge record must cover the entire period during which the water quality samples were collected. There must be a date and analyte concentration for each sample in the record. Time of day information is not used in EGRET. The analyte concentrations may be censored values. These include left-censored data (for example "less than 0.1 mg/L") but also interval-censored data (for example "less than 1.1 mg/L but greater than 1.0 mg/L"). The graphics produced can be very useful in characterizing how the analyte concentration relates to discharge, how it varies by season, and how it may be changing over a period of years. These simple empirical descriptions are often useful to help support results

produced by rather complex methods of analysis such as those conducted in the third component of EGRET.

3. This third component of EGRET involves applying the Weighted Regressions on Time, Discharge, and Season (WRTDS) smoothing method (Hirsch and others, 2010) to interpret the behavior of the water quality analyte of interest on the basis of four components: the relationship to discharge, seasonality, long-term trend, and a random component. This analysis produces tabular and graphical representations of the concentration and the flux of the analyte as it relates to these driving factors. It presents annual and seasonal summaries of the behavior of concentration and flux over time but also presents flow-normalized estimates of concentration and flux which are designed to remove the influence of year-to-year variations in discharge and thus provide more insight on underlying changes in the behavior of the watershed. This component also provides a wide range of specialized graphics aimed at identifying potential problems of bias in flux estimates (Hirsch, 2014) and describing the nature of the changes that have taken place. For example, it can identify changes that are specific to base flow or high flow conditions and/or particular seasons of the year.

Organization of this report

This report begins with a description of the options for entering each of the three primary data types used by EGRET. These three data types each have a specific type of data frame that organizes all of the data entered and contain outputs that are computed from those data. The names of these three data frames are: `Daily`, `Sample`, and `INFO`. A data frame in R is a two-dimensional matrix (a table), in which each column is a variable (with its own name and data type) and each row is a specific observation. Having a general understanding of the three primary data frames is very valuable to the user. Knowing what is stored in these data frames and what the variables are named makes it possible

for the user to employ other statistical or graphic functionality that exists in R. For each of these three data frames this report provides an explanation of how to use the dataRetrieval package to enter the relevant data (discharge data, water quality data, and metadata). This is followed by two brief sections. The first of these explains how EGRET handles the definition of seasons and years (called the "Period of Analysis") and the second of these explains how EGRET handles units. This is followed by sections covering each of the three components of EGRET discussed above: flow history, summarizing water quality data (without using WRTDS), and WRTDS analysis of water quality data. Each of these sections describe the concepts and mathematics involved, identifies the specific EGRET functions that are available in the package, and provides illustrations of the types of outputs they produce. Near the end of the report are shorter sections dealing with editing data sets, working with multiple data frames, and batch processing.

Getting help with functions

It is assumed that the reader of this report has a rudimentary knowledge of the R language and environment. General information on R can be obtained from the R-project at *http://www.r-project.org/* (particularly the Manuals page). There are also many texts that teach about the use of R.

Detailed directions on the use of individual functions, with the full range of user options are presented in Appendices A and B for the dataRetrieval and EGRET packages respectively. These appendices are also known as vignettes and they follow a standard format used for R packages. In addition, very detailed descriptions of all of the functions contained in both packages are available to the user within the R software environment once the dataRetrieval and EGRET packages have been loaded onto the user's computer. For example, information about the function `getSampleData` in the dataRetrieval package can be obtained with the command `?getSampleData`.

Users will note from the appendices that most of the functions in dataRetrieval and EGRET have a very large number of arguments, most of which have default values. This is particularly true for all of the graphics functions. The graphics functions are designed to offer a great deal of flexibility in terms of size of characters, set-up of axes and their labels. However, they were all designed in such a way that the default settings create a highly presentable graphic for purposes of reports and presentations. The body of this user guide will not delve into most of these arguments. Users who want to make adjustments are directed to the help pages and the EGRET vignette (appendix B) for instructions for using them. In most cases, a function that produces a graph or a table can be used simply by typing its name followed by ( ). Examples of commands given in this report will generally specify a minimal set of arguments and ignore many of the arguments used for detailed settings of graphics. Most of the functions described have arguments that specify names of data frames. These typically look like this: `localDaily = Daily, localSample = Sample, localINFO = INFO`. For most purposes users can ignore these arguments and just allow them to be set at their default values (and as a consequence they don't need to be specified in the actual command line). Advanced users may want to create alternative versions of these and other data frames to make various types of comparisons. This kind of advanced use in described in the section of the report entitled "Working with multiple versions of data frames".

The information in this report and the Appendices are written to describe the interactive use of the software. However, as is generally the case in R, batch processing is easily done by creating a file of specific commands to be executed. Once the proper workflow for a particular project has been established, this file of instructions can be input to the R environment on the user's computer and the computations can proceed without the need for repeated steps by the user. Suggestions for batch processing are provided in a section titled "Batch processing in EGRET" near the end of the user guide. Another important feature of R is that all of the code in the basic R package as well as these two specific

packages described here is freely available to the user. For example, to see the code for the function `getSampleData` the user simply can enter `getSampleData` (without parentheses) at the R-command line and the complete code will appear on the user's console, from which it can be freely copied. This means that users who want to develop their own R applications that have some similarity to those in the dataRetrieval and EGRET packages can examine the code and then copy and modify it to suit their own needs. There are no copyright restrictions on any of the basic R codes or any aspects of these two packages.

Package Installation

Installing the packages involves first installing the packages that dataRetrival and EGRET depend on, then installing the packages themselves. For Mac and Windows users, the commands are simply:

```
install.packages(c("zoo","survival","methods","fields",
      "spam","XML","RCurl","plyr","reshape2"))
install.packages(c("dataRetrieval","EGRET"),
      repos="http://usgs-r.github.com/")
```

Unix users will need to add `type="source"` to both commands. Once this report is published, the packages may be moved to the CRAN repository (Comprehensive R Archive Network). This will allow the package to be installed with all required dependencies simply with the command:

```
install.packages(c("dataRetrieval","EGRET"))
```

Data Entry

Overview of data entry

In the examples to follow, we will consider the example of a streamgage (Choptank River near Greensboro, MD) with USGS site ID 01491000, and we will look for daily mean discharge and sample

values of dissolved nitrate plus nitrite which has parameter code 00631. It is assumed here that the user already knows the unique identifier of the streamgage and the desired parameter code. Data discovery is not the focus of this software or report. There are a number of data discovery tools that can facilitate finding sites within some region that may meet the users data requirements. For example, the NWISweb system (*http://waterdata.usgs.gov/nwis*) allows a user to discover sites with a specified minimum amount of data (for example a minimum number of mean daily streamflow values or a minimum number of water quality samples). The dataRetrieval package provides a capability to use several types of data sources. The body of this report will focus only on those functions needed to retrieve data for the EGRET package. However, these functions and some other functions in dataRetrieval have much broader applicability for retrieving a variety of USGS and other agency data. These are summarized in table 8 of the Summary section in appendix A.

Mean daily discharge data for use in EGRET

The EGRET software requires that there be a continuous record of mean daily discharge data for the study period. In those cases where only flow history analyses are being done the user may want to obtain the entire record, or if the study period has a standard starting and ending date then these dates can be used. In the case of a WRTDS water quality study, the period over which the WRTDS model will be estimated is defined entirely by the user's selection of the starting and ending dates of the daily discharge data. These dates must completely span the period of record of the water quality data that will be used in the analysis. In other words, the discharge record being used must start on, or before, the first sample day, and end on or after the last sample day. However, the daily discharge record should not extend more than a few months beyond the range of the water quality record. Using a discharge record that extends far beyond the period of water quality record will cause WRTDS to perform extrapolations. WRTDS is a smoothing method and, as such cannot be expected to produce meaningful extrapolations

in time. Estimates for dates a few years beyond the water quality record can be totally unrealistic. Thus, a good practice would be to select a starting date that is the beginning of the first water year in which there are water quality data and an ending date that is the last day of the last water year in which there are data. It is acceptable to have starting and ending dates that are not the start or end of the water year, but the user's choice of these dates, along with their choice of the whether annual results are to be presented on a water year or calendar year or seasonal basis, will influence whether or not the first and/or last years of the analysis will be reported.

The mean daily discharge data are stored in EGRET in a data frame called `Daily`. It has a very specific structure and naming convention for all of its columns, although users can always add columns as needed. Table 1 describes the contents of the `Daily` data frame. The number of rows in the data frame is equal to the number of days in the mean daily discharge record. Initially, the number of columns is 11. However, once the WRTDS computations have been run using the `modelEstimation` function, the data frame is automatically augmented with an additional 6 columns computed by that function (as described below in the section "WRTDS analysis of water quality data").

Table 1. A list of the column names for the `Daily` data frame. Those shown in black are computed from the date and discharge information retrieved and stored when the data frame is created. Those in red are created and stored automatically when the WRTDS computations are made by the EGRET package using the `modelEstimation` function.

Name	Definition	Data type	Units
`Date`	The date	Date	yyyy-mm-dd
`Q`	Mean daily discharge on that date	numeric	m^3/s
`Julian`	The date expressed as days starting with Jan 1, 1850	numeric	days (integer)
`Month`	Month of the year, from 1 to 12	numeric	months (integer)
`Day`	Day of the year, from 1 to 366	numeric	days (integer)
`DecYear`	Year expressed as a decimal	numeric	years
`MonthSeq`	Month sequence: an index starting with 1 at Jan, 1850	numeric	months (integer)
`LogQ`	ln(Q)	numeric	dimensionless
`i`	index of days from the start of the data frame	numeric	days (integer)
`Q7`	Mean discharge for 7 days, up to day i	numeric	m^3/s

Q30	Mean discharge for 30 days, up to day i	numeric	m^3/s
yHat	The WRTDS estimate of the log of concentration	numeric	dimensionless
SE	The WRTDS estimate of the standard error of yHat	numeric	dimensionless
ConcDay	The WRTDS estimate of concentration	numeric	mg/L
FluxDay	The WRTDS estimate of flux	numeric	kg/day
FNConc	Flow normalized estimate of concentration	numeric	mg/L
FNFlux	Flow normalized estimate of flux	numeric	kg/day

The variable Q7 is the mean discharge for the 7 days up to and including the specific day for that row (e.g. for September 21, 2010 Q7 would be the average of the discharge values for September 15-21, 2010). Q30 is the mean for the 30 days up to and including the specific day for that row. Note that at the start of the record there will be 6 missing values for Q7 (designated as NA) and 29 missing values for Q30. There are two ways to obtain the discharge data, either from USGS data services or from a user-supplied data file.

Discharge data from USGS data service

For those cases where the discharge data are from the USGS, obtaining the data from a web service retrieval is the preferable approach to obtaining the data. The source for these data is the USGS data service at: *http://waterservices.usgs.gov/*.

The function used to obtain the daily discharge data is getDVData. In the case of the Choptank River example, the set of commands would be as follows:

```
siteNumber <- "01491000"
QParameterCd <- "00060"
StartDate <- "1979-10-01"
EndDate <- "2012-09-30"
Daily <- getDVData(siteNumber, QParameterCd, StartDate, EndDate)
```

Alternatively, one could proceed without defining the four arguments to the function and enter them directly into the function call, which would then look like this:

```
Daily <- getDVData("01491000","00060","1979-10-01","2010-09-30")
```

This command instructs the users' computer to retrieve the daily mean discharge data from a specified USGS URL, make the necessary computations to create the Daily data frame for the specified

streamgage and period of record. The command will also return some information about the length of the record, gaps that may exist, and the presence of zero or negative discharge days. The second argument value in the `getDVData` function for an EGRET application should always be `"00060"` (which is discharge in cubic feet per second). `getDVData` will convert the cubic feet per second data to cubic meters per second by default. However, the `getDVData` function is designed so that it could be used to retrieve other parameters that are stored in a daily values format for analyses that are outside the scope of the EGRET package. In such cases if one is using a different parameter code than `"00060"`, be sure to also include the argument `convert=FALSE` in the command, otherwise a conversion factor will be applied. A list of some common parameter codes for daily data available from the USGS are given in Appendix A, Table 1. Users interested in obtaining other types of daily data should refer to Appendix A.

If the user is uncertain about what the starting and ending dates should be, or wants to retrieve the entire period of record, the command could be:

```
Daily <- getDVData("01491000","00060",StartDate="",EndDate="")
```

This will result in a record that contains all available mean daily discharge data for the requested streamgage. It is not uncommon for the final few weeks or months of the record to contain missing values. The program will return information to the console telling how many days there are between the first and last days of the record and how many daily values there are. If the number of daily values is smaller than this time span it will also state the starting and ending date of the gaps. This information can help the user determine how to shorten the total period requested in order to obtain a record with no gaps. If there are gaps, the user will need to modify the `StartDate` and/or `EndDate` to avoid having gaps in the record. In a water quality data analysis project it may be necessary for the user to iterate between the discharge data retrieval and the water quality sample retrieval in order to obtain an appropriate period of record for both. Doing this will require rerunning the `getDVData` function. Each

time the function is called it will simply overwrite the previous version of the `Daily` data frame with the new one. The user does not need to delete the earlier version of `Daily`.

Data in the record may be denoted as “P” (Provisional) or “A” (Approved) in the `Daily$Qualifier` column. The more recent portion of the record may contain provisional data, whereas the older data will have been through the USGS approval process. The following series of commands will enable the user to identify the span of dates for which the reported data are Provisional.

```
DQ <- subset(Daily,Qualifier=="P")
```

This command simply creates a new data frame from the `Daily` data frame, selecting only those days for which the Qualifier is "P".

```
summary(DQ$Date)
```

This command will return a summary of the dates in `DQ` showing the first and last provisional date. If the user does not want to use provisional discharge data the following command will remove the rows with provisional data:

```
Daily <- subset(Daily,Qualifier!="P")
```

The user may want to clean up their workspace at this point by removing the data frame `DQ`. The command is:

```
rm(DQ)
```

The `getDVData` function will also report the number of days of zero or negative discharge. Negative discharge values can arise at sites with backwater conditions. Because many of the computations in EGRET use the natural log of discharge there cannot be any zero or negative discharge days in the record. The presence of even one zero or negative discharge values will cause the EGRET calculations to fail. If there are any zero or negative values, these will all be set to zero and then a very small constant will be added to all of the discharge data. This constant is set to 0.1% of the mean discharge in the record. If there are a very small number of zero or negative flow days (for example less

than 0.2% of the days) there should be no serious problems in using EGRET. But, if there are large numbers of zero or negative flow days, the statistical methods will probably be compromised by having a large number of days all having values tied at this arbitrary minimum value of discharge. Final numerical results from EGRET should have this small flow increment subtracted out of discharge and flux results, but typically these adjustments would be so small as to have no consequence if users are reporting results to an appropriate number of significant figures.

Once the data are retrieved the data set can be explored with the command:

```
summary(Daily)
```

It will report the time span of the data set and the range of the data values. Note that the discharge values in the summary are automatically converted to m^3/s, the discharge units used for all calculations in EGRET, but for all of the specific graphical and tabular output functions of EGRET the user will have a choice of four different units in which to report discharge (see subsequent section "Selection of units of measurement for graphs and tables in EGRET").

The total number of mean daily discharge values can be obtained by giving the command:

```
length(Daily$Q)
```

And a very simple plot of the time series can be obtained with the command:

```
plot(Daily$DecYear,Daily$Q,log="y",type="l")
```

Note, in type="l" that is a lower case letter L. It stands for "line". When type is not listed, the plot function's default symbol is a point rather than a line. Looking at the summary and at such a time series plot is a good opportunity to spot data problems that may need to be resolved.

Discharge data from a text file

If the discharge data are not available from USGS data services, but they are available in the form of a spreadsheet, then they can be entered as comma-separated values (usually denoted with a

".csv" extension). The option of using other file types is discussed in more detail in Appendix A. The file must consist of two columns. The first is the date expressed as mm/dd/yyyy or yyyy-mm-dd. The second column is daily discharge. A common error is the use of a two-digit year (e.g. 04/25/12). Spreadsheet programs tend to revert to these two-digit years, even though they are ambiguous. The first row in the file should contain headings such as "date" and "Qdaily" although the choice of names is of no consequence.

The user must define two variables to identify the full name of the data file. The first of these is called `filePath` and the second is called `fileName`. The variable `filePath` is a character string that defines the path to the file on the user's computer. This can either be a full path name, or path relative to the R working directory, and should end with '/'. Windows user should be aware that R requires paths to use the forward slash ('/'), whereas Windows tends to use the backwards slash ('\') in many other applications. Using the backwards slash will cause an error. No matter what operating system is being used, the forward slash is required in R. The variable `fileName` is a string that defines the file name (including the extension).

As an example, for the MacOS:

```
filePath <- "/Users/rhirsch/desktop/"
fileName <- "ChoptankFlow.csv"
```

Once those two variables are defined the function can be called: In its simplest form it would be:

```
Daily <- getDailyDataFromFile(filePath, fileName)
```

The default case is that the discharge values in the file are in units of ft^3/s. The alternative is that they are expressed in m^3/s. If that were the case then the command would be:

```
Daily <- getDailyDataFromFile(filePath, fileName, qUnit = 2)
```

If the spreadsheet available provides discharge in some other units (say L/s, or gal/hr) the user will have to make a conversion in their spreadsheet program to convert them to either m^3/s or ft^3/s. The same

rules regarding the starting and ending date of the record apply here as were described above but they are set simply by the user editing the data file to have the appropriate starting and ending dates. The function `getDailyDataFromFile` checks for zero and negative discharge values and makes the necessary changes to the data set as are as are described above for the function `getDVData`.

Water quality data for use in EGRET

Water quality data are stored in EGRET in a data frame called `Sample`. It only contains information about one analyte, although it may be that this analyte is computed as the sum of two or more analytes (see discussion below). It has a specific structure and naming convention for all of its columns, although users can always add columns. Table 2 describes the contents of the `Sample` data frame. The number of rows in the data frame is equal to the number of sample values in the data set. Initially, the number of columns is 14. However, once the WRTDS computations have been run using the `modelEstimation` function, the data frame is automatically augmented with an additional 3 columns computed by that function (as described below in the section "WRTDS analysis of water quality data").

Table 2. A list of column names for the Sample data frame. Those shown in black are computed and stored when the data freame is created. Those in red are created and stored automatically when the WRTDS computations are made by the EGRET package using the `modelEstimation` function.

Name	Definition	Data type	Units
`Date`	The date of the sample	Date	yyyy-mm-dd
`ConcLow`	Lower bound for an observed concentration	numeric	mg/L
`ConcHigh`	Upper bound for an observed concentration	numeric	mg/L
`Uncen`	=1 if sample is uncensored, =0 if censored	numeric	integer
`ConcAve`	Average of ConcLow & ConcHigh	numeric	mg/L
`Julian`	The date expressed as days starting with Jan 1, 1850	numeric	days (integer)
`Month`	Month of the year, from 1 to 12	numeric	months (integer)
`Day`	Day of the year	numeric	days (integer)
`DecYear`	Year expressed as a decimal	numeric	years
`MonthSeq`	Month sequence: an index starting with 1 at Jan, 1850	numeric	months (integer)
`SinDY`	sin(2*π*DecYear)	numeric	dimensionless

CosDY	cos(2*π*DecYear)	numeric	dimensionless
Q	Mean daily discharge on the day of observation	numeric	m^3/s
LogQ	Natural logarithm of Q	numeric	dimensionless
yHat	cross-validation estimate of the log of concentration	numeric	dimensionless
SE	cross-validation estimate of the standard error of yHat	numeric	dimensionless
ConcHat	cross-validation estimate of concentration	numeric	mg/L

The Sample data frame is designed to accommodate censored data. Typically, when the concentration is very close to zero the laboratory will report it as "less than" some reporting limit. In the USGS NWIS database this is communicated through a remark code of "<" followed by a value which is typically set to the reporting limit. The dataRetrieval package structures the concentration data in the Sample data frame in a manner that will make them suitable for use in the survival regression, which is the statistical method used by WRTDS. The concentration information is stored using two variables, one called ConcLow and the other called ConcHigh. When the data are uncensored, these two will be equal to each other (set to the reported concentration value). If a value is censored, for example with a reporting limit of 0.5 mg/L, then ConcLow will be set to NA (which stands for Not Available) and ConcHigh will be at the reporting limit, in this case 0.5. The variable called Uncen is always 1 for an uncensored value and 0 for a censored one. The mean value of Uncen for any given data set will be equal to the frequency of uncensored values in the data set. For example if the mean of Uncen is 0.95, then 95% of the values are uncensored and thus 5% of the values are censored. The variable ConcAve is provided for convenience and is used in some of the graphics functions but is not used in any computation. For censored values where ConcLow is equal to NA, ConcAve it is set equal to 0.5*ConcHigh. This type of censoring is referred to in the statistical literature as left censoring.

The Sample data frame structure is designed to also handle the more complex case of interval censoring. The following is an example of one of the ways that interval censoring can arise. In the Chesapeake Bay River Input Monitoring Program (Moyer and others, 2012, pp. 4,6,9–11) there is a set of rules for computing total nitrogen as the sum of multiple individual nitrogen analytes. The rule that

applies to the data collected at the Potomac River at Chain Bridge, Washington, DC for the year 1999 is that total nitrogen is computed as the sum of two analytes that were measured at that time: One is nitrate plus nitrite, filtered (USGS parameter code 00631) and the other is ammonia plus organic nitrogen, unfiltered (USGS parameter code 00625). Consider the sample from June 7, 1999. The nitrate plus nitrite was reported as 0.596 mg/L and the ammonia plus organic nitrogen was reported as <0.1 mg/L. The sum of these two values lies in the range 0.569 mg/L to 0.696 mg/L. Using the convention adopted for the `Sample` data frame the `ConcLow` value would be 0.569 and the `ConcHigh` value would be 0.696 and the variable `Uncen` would be equal to 0. Because this situation (where two or more analytes are summed to form the variable of interest) is somewhat uncommon, the details of data entry for these cases are presented in Appendix A section 3.4 rather than here in the body of the report.

There are two other instances where the interval censoring approach may prove useful. One is to deal with changes in rounding of reported concentrations. It is not uncommon to see a set of concentration data in which the later part of the record are reported with more significant figures than those in the earlier part of the record. If one is concerned about the possibility that the change in rounding practices may influence the results of the subsequent analysis, it may be useful to code the more rounded values to be represented as interval censored. For example, consider a case where the data are reported as 0.01, <0.01, 0.03, and 0.02 but after the fourth value the laboratory changes its reporting conventions so that more significant figures are reported and the next three values in the same data set were reported as 0.0134, 0.0545, 0.0252. Using the reporting conventions used in EGRET one might want to report these seven observations as follows with each represented by a `ConcLow`, `ConcHigh` pair of values: (0.01, 0.015), (NA, 0.01), (0.025, 0.035), (0.015,0.025), (0.0134,0.0134), (0.0545,0.0545), and (0.0252,0.0252). The process of creating these intervals is described below in the section “Editing data sets”.

Yet another application of interval censoring could be used to modify concentration values for which there is an unusually large amount of uncertainty. For example, a measurement made in flood conditions where the sample collection method could have resulted in a biased sample. If the analyst is prepared to indicate an upper and lower bound on what might be the true value for the sample, then these can be substituted for `ConcLow` and `ConcHigh`. Using these interval estimates can be a useful sensitivity check to learn if a few highly uncertain but highly important samples could have a large influence on the final analysis of long-term fluxes or trends. These types of changes are also described below in the section "Editing data sets".

Water Quality Data from USGS Web Services

To obtain the water quality data from the USGS Data Services, all that is needed is a station number, parameter code and a starting and ending date. The function used to obtain the data is `getSampleData`. In the case of the Choptank River, for the parameter nitrate plus nitrite, filtered, reported as N, (parameter code 00631), and assuming that we wanted sample values from water years 1980 through 2012 the set of commands could be as follows:

```
siteNumber <- "01491000"
ParameterCd <- "00631"
StartDate <- "1979-10-01"
EndDate <- "2012-09-30"
Sample <- getSampleData(siteNumber, ParameterCd, StartDate, EndDate)
```

or, alternatively, one could proceed without defining the four arguments to the function and enter them directly into the function call, which would then look like this:

```
Sample <- getSampleData("01491000","00631","1979-10-01","2010-09-30")
```

Another approach, when the analyst is unsure of the time period for which sample data are available would be to give the command in this manner.

```
Sample <- getSampleData(siteNumber, ParameterCd, StartDate="", EndDate="")
```

This will return all data for that site and parameter. To determine what the first and last sample dates are, the user can give the command:

```
summary(Sample)
```

The first column will show the first and last dates. Note that at this stage of the process, there will be no columns in the `Sample` data frame for `Q` or `LogQ`. These will be created later using the function called `mergeReport` which obtains the discharge data from the `Daily` data frame.

There are times when the data set has just a few values in the early years and then denser sampling commences at a later date. The user may wish to eliminate the early part of the record from the analysis because the data are so sparse or a gap is too long. An easy way to identify this type of situation is with a simple plot.

```
plot(Sample$DecYear,Sample$ConcHigh)
```

This plot will show if there are large gaps in the sampling record. Based on that, the analyst might choose to adjust the request by the choice of a more restrictive set of values for `StartDate` and `EndDate`. Depending on what dates are chosen it may be necessary to return to the `getDVData` function to obtain a discharge data set that fully covers the sample data time period but does not extend far beyond the first and last sample dates. Large data gaps (such as two or more years of no data) should be noted. The WRTDS analysis can be run on data sets with gaps of several years in the water quality record. The results during the gap period will be highly unreliable, but the results on either side of the gap period will be quite reliable. Once the WRTDS analysis is completed (using `modelEstimation`) the results can be modified to remove the results from the data gap period using the function `blankTime`, which is described in the section on WRTDS analysis.

Water Quality Data from EPA STORET Data Service

In addition to obtaining water quality sample data from the USGS, dataRetrieval can also obtain EPA STORET data from the Water Quality Data Portal (*http://www.waterqualitydata.us/*). The retrieval process is very similar to that described above for the function `getSampleData`. In this case the function is called `getWQPData`. The first argument is a station identifier and the second is a "characteristic name." This is an example of a retrieval for specific conductance data for a site in STORET operated by the Department of Natural Resources in Wisconsin.

```
Sample <- getWQPData("WIDNR_WQX-10032762","Specific conductance", "", "")
```

Site names begin with an identifier of the data source (such as a State agency database), followed by "_WQX-" followed by the identifier within the original data source. Guidance on finding characteristic names can be found at: *http://www.waterqualitydata.us/Codes/Characteristicname*.

Water Quality Data from a User Supplied File

If the water quality data are not available from one of these data services, they can be entered from a user-supplied file. Just as in the case of the discharge data from a user-supplied file, the user will have to supply a specific `filePath` and `fileName`. For example, on a MacOS these could be:

```
filePath<-"/Users/rhirsch/Desktop/waterqualitydata/"
fileName<-"ChopNO3"
```

The default structure of the file is a csv file (comma separated values) although other structures such as tab delimited or space delimited are possible. The default structure also expects column headings for each column. There are alternatives to this default structure, these are described in Appendix A (section 3.5.2) and in the help for the `dataRetrieval` function `getSampleDataFromFile`. In the default case, each column needs a header in the first row. They can be called something like "date" "remark" and "value" (but alternative names will work). The first column must contain the sample date, which should be in the form mm/dd/yyyy or yyyy-mm-dd. Two-digit years are not

acceptable because they are ambiguous. The second column is for the remark. The column is required even if there are no remarks. This column should show "<" for all less-than values, and be blank otherwise. The third column is the concentration. In the case where there is a "<" in the remark column the concentration column should contain the reporting limit. It is assumed that all concentrations are in mg/L. There should never be a zero value in the concentration column. The function will look for that, and if it exists it will give a warning and discard it. If this situation arises, the original data set should be reviewed and a proper interpretation of the zero values should be determined if possible. They should be re-coded in the original data set, preferably to have a "<" in the remark column and the zero replaced with a reporting limit in the value column. In cases where the analyst cannot determine what the correct reporting limit should be, some reasonable convention may be used, such as setting these values to some number less than the lowest reported value. This type of approximation is likely to be better than leaving the value at zero and or deleting the observation. These alternatives can result in a serious bias. In the more complex case, where the variable of interest is the sum of multiple analytes, the input file can contain more than three columns. For each additional analyte there will be a remark column followed by a value column. The function will sum analytes across all the columns to come up with the concentration value that is used. The presence of these additional pairs of remark and concentration values will cause the program to compute concentrations as the sum of the analytes included. For details, refer to Section 3.4 of Appendix A.

Entry and storage of meta-data

Meta-data about the site and the analyte being evaluated are stored in a data frame called `INFO`. Depending on the way in which meta-data are acquired, there can be a large number of data elements in `INFO`. These are listed in Appendix A. There are only a few items of meta-data that are required for the EGRET functions to run. These are shown in Table 3.

Table 3. Variables required in the INFO data frame for use in EGRET applications.

Variable name	Definition	Purpose
shortName	Name of data collection site	Name of site used in all graphs and tables
paramShortName	Name of the parameter (or constituent)	Name of parameter as used in all graphs and tables
staAbbrev	Abbreviated name of site	Abbreviation used to name files storing workspaces for the site
constitAbbrev	Abbreviated name of parameter (or constituent)	Abbreviation used to name files storing workspaces for the parameter (or constituent)
drainSqKm	Drainage area at the monitoring site in km^2.	Used to compute runoff (e.g. in mm/d) or yields (e.g. in $kg/y/km^2$)

Regardless of the source of metadata, they are entered into the system by using the function `getMetaData` with just two arguments, `siteNumber` and `parameterCd`. In the case where all of the data comes from a USGS data service call, the command for USGS site number 0149100 and parameter number 00631 would be:

```
INFO <- getMetaData(siteNumber = "0149100", parameterCd ="00631")
```

Or equivalently

```
INFO <- getMetaData("0149100", "00631")
```

If the application were one only dealing with discharge data and not water quality, the command would be:

```
INFO <- getMetaData(siteNumber = "0149100", parameterCd = "00060")
```

If the site is not one in the USGS database then the first argument would be "" and if the USGS parameter code was unknown the second argument would be "". Thus, in the case where there is no USGS site number and no USGS parameter code the function call would be:

```
INFO <- getMetaData("", "")
```

In cases where site and/or parameter codes don't exist, the `getMetaData` function will request inputs from the user. The only responses that must be supplied are those listed in Table 3.

The `getMetaData` function populates the `INFO` data frame from the meta-data that it acquires from USGS data services where that is possible, using the station number and parameter code. In general this is an interactive process, and `getMetaData` provides a series of prompts to the user requesting user input. The specific prompts depend on the information provided in the call to the function. The following are some of the items that are requested and the reasons for them.

- Station name: When a station number is supplied the prompt provides the user with the exact name of the station in the USGS database. First, the user should check to see if this is actually the site they intended. Assuming it is, the user has the option to enter the station name in a different form, chosen to provide the most readable and informative rendition of the name, as it will appear on all figures and tables. This option is available because in some cases the station name as provided is not particularly suitable for use in figure or table titles. For example some stations have names that are in all capital letters, which can be difficult to read. The user can type in a version that uses upper and lower case letters. Sometimes the site name is exceedingly long, and the user may want to shorten it to make it more suitable for use in graphs and tables. If the user is satisfied with the name as provided, all that is needed is a carriage return and it will be used. The original official USGS station name is retained in the `INFO` data frame so that if there is any doubt about the official name it remains available.
- Parameter names: Similarly, parameter names can be very long and complex, and thus, not suitable for use in titles of figures or tables. If the parameter code is provided in the call to `getMetaData` this full name is provided and then the user is prompted to provide a shorter alternative more suitable for use in figures and tables. If the original wording is acceptable, then all that is needed is a carriage return. Again, the official name of the parameter is retained in the `INFO` data frame.

- Station and parameter abbreviations. The `getMetaData` function will prompt the user for abbreviations. These can be very helpful to the user for managing the various files involved in a larger project (with many sites and many parameters). The user should develop their own lexicon of simple abbreviations for their sites (e.g. the Choptank site could be "Chop" and the nitrate parameter could be "NO3"). Files that the user may create and update in the course of the project are automatically named through the use of these abbreviations. (See the section "Saving the workspace for future use"). So, for example the workspace containing the Choptank River Nitrate example would be called "Chop.NO3.RData". This can be very helpful in structuring large batch jobs as well as for returning to a previous data analysis.
- Drainage area. If the site is in the USGS database then there should be a drainage area stored. It will typically be in mi^2. The prompt will give this information and will show the value converted to km^2 (both numbers are stored). But if there is no known drainage area, the user will be prompted to provide one and the units in which they provided it (mi^2, km^2, acres, or hectares). If the user has no way of knowing the drainage area they should respond by entering the number 0. As a consequence, attempts to compute runoff in units of mm/day will fail (as they should) and generate an error message.

There are many additional metadata elements that will be stored in `INFO` of they are available from the user or from data services. In R, typing the name of an object results in the entire content of the object being sent to the user's console, thus users can review all the metadata that are stored in `INFO` just using the command:

```
INFO
```

Moving discharge data from the Daily data frame to the Sample data frame

All graphics and analysis in EGRET that relate to water quality require that every sample value have associated with it a mean daily discharge value for the day on which the sample was taken. To assure consistency between the `Daily` and `Sample` data frames, these data are imported from the `Daily` data frame to the `Sample` data frame. The function that accomplishes this is called `mergeReport`. For convenience, in addition to the importing that it accomplishes, it provides a compact table of information about the contents of both the Sample and Daily data frames. The call to the function is:

```
Sample <- mergeReport()
```

It returns the original `Sample` data frame, augmented with the two columns `Q` and `LogQ` which are the mean daily discharge on the sample date and the natural log of that discharge. Figure 1 is an image of the report provided in the Choptank nitrate example.

```
Discharge Record is 12631 days long, which is 35 years
First day of the discharge record is 1978-10-01 and last day is 2013-04-30
The water quality record has 632 samples
The first sample is from 1979-09-25 and the last sample is from 2013-04-29
Discharge: Minimum, mean and maximum 0.00991 4.13 246
Concentration: Minimum, mean and maximum 0.04 1.1 2.4
Percentage of the sample values that are censored is 0.32 %
```

Figure 1: Example of the output from the mergeReport function.

Removing duplicate observations

There are cases where there may be multiple observations from a single day that have identical sample values and the user wishes to remove the duplicates. The call to the function that would carry out this process is:

```
Sample <- removeDuplicates()
```

This command will edit the Sample data frame to eliminate such duplicates.

Saving the workspace for future use

Once the `Sample`, `Daily` and `INFO` data frames have been created it is recommended that the user save the workspace for future use in the EGRET software. What is needed to do this is to define the variable `savePath`, which indicates the full pathname in the computer's file structure where one wishes to store this workspace. The user will have to supply that pathname. For example, on a MacOS these could be:

```
savePath <-"/Users/rhirsch/Desktop/myWorkspaces/"
```

Note the "/" at the end of the name. It is required. Then, to execute the command and save the workspace the command would be:

```
saveResults(savePath)
```

The result of this (using the `staAbbrev` and `constitAbbrev` examples used above) would be that there would now be a file called: `/Users/rhirsch/Desktop/myWorkspaces/Chop.NO3.RData`. At any time in the future this workspace can be restored simply by giving the command:

```
load("/Users/rhirsch/Desktop/myWorkspaces/Chop.NO3.RData")
```

Depending on the operating system or specific version of R being used, this can alternately be accomplished from a drop-down menu or by dragging the icon for the file into the console. Users can experiment to find the simplest ways to do this for their implementation of R. During the further analysis of the data set, users should use the `saveResults` function repeatedly so that the analysis completed can be stored for future use. In some cases, users may wish to save different versions of the same data set. They may differ in terms of the length of the data set used, some change in the handling of censored values, or some differences in the settings used in conducting certain analyses. These separate versions of the workspace can be stored by creating new abbreviations and then storing the workspace again with the `saveResults` function.

For example, say we choose to look at a different version of the Choptank River Nitrate data set, one that is truncated at the end of water year 2007. We could create that workspace by using `EndDate="2007-09-30"` in both the `getSampleData` and `getDVData` functions. Then, when the `getMetaData` function is used the user could specify (in response to the prompt) that the `stationAbbrev` could be ChopShort. Then when the `Sample`, `Daily` and `INFO` data sets have been created, and the `mergeReport` function has been run, the user can simply give the command `saveResults(savePath)` and the new data frame would be automatically named `/Users/rhirsch/Desktop/myWorkspaces/ChopShort.NO3.RData`

Alternatively, once some modification of an analysis has been carried out, the user can directly modify one or both of the abbreviations. For example if an alternative analysis is carried out, the user could specify a different value for `consititAbbrev` and/or `staAbbrev` and that would determine the name given to that workspace.

```
INFO$constitAbbrev <- "NO3version2"
INFO$staAbbrev <- "ChopOriginal"
saveResults(savePath)
```

The result of these commands would be the saving of a file called:

```
/Users/rhirsch/Desktop/myWorkspaces/ChopOriginal.NO3version2.RData
```

Setting the period of analysis for graphs, tables, and analyses in EGRET

Many hydrologic studies (whether of streamflow or of water quality) need to provide results that are specific to a particular part of the year rather than the entire year. Also, for different audiences, the representation of a year that they are accustomed to seeing may differ. Some audiences want to see the water year (October through September) while others may want to see the calendar year. Throughout the EGRET software, both for flow history studies as well as water quality studies, the necessary flexibility to show different seasons or different definitions of a year are provided through the concept

of the "period of analysis" or "PA". If the outputs are reported by water year, then the PA is October through September. If the outputs are calendar years then the PA is January through December. If the output is for the winter season, as defined by the months of December, January and February then those 3 months become the PA. If the outputs are only for the month of May then the PA is May. The only constraints on the definition of a PA are these: 1) It must be defined in terms of whole months. 2) It must be a set of contiguous months (like March-April-May). 3) It must have a length that is no less than 1 month and no more than 12 months. The PA is uniquely defined by two arguments: `paLong` and `paStart`. `paLong` is the length of the period of analysis in months, and `paStart` is the first month of the PA (using the calendar year, so January is month 1). Table 4 summarizes `paLong` and `paStart` through a series of common examples.

Table 4. Examples of the Period of Analysis and the paStart and paLong values associated with them.

Period of Analysis	paStart	paLong
Calendar Year	1	12
Water year	10	12
Winter (December - February)	12	3
Warm season (May-September)	5	5
September	9	1

Virtually all of the EGRET functions that provide graphs or tables of the data or statistical results have the capability to restrict their output to be related to some particular PA. The only exceptions to this are the functions: `plotConcQSmooth, plotConcTimeSmooth, plotContours, and plotDiffContours`. The defaults are always `paStart = 10` and `paLong = 12` (the water year) and all graphics and tables produced by EGRET that use a PA will indicate what PA was used to produce them.

The year listed in any tabular output from EGRET is the calendar year at the time the PA ends. This is the same approach used for numbering water years. The water year starting October 1, 1990 is called water year 1991. If the PA were `paLong` = 6, `paStart` = 9 (a period running from September

through February) the results for the period September 1, 2000 through February 28, 2001 would be listed as the 2001 value.

The annual values shown on any EGRET graphic are always plotted at the mean date for the period (expressed in decimal years). Thus, a calendar year average would be plotted at the mid-point of the calendar year. So for calendar year 1981, the mean value would be plotted at 1981.5. For a water year, the mean value would be plotted at the mean date for the water year. So for water year 1981 the mean would be plotted at 1981.25. If the PA were `paLong` = 4 and `paStart` = 3 (a period consisting of the months of March through June) then the mean value for 1981 would be plotted at 1981.33 (which is May 1, 1981). The tick mark on the graph for a given year is plotted on January 1 of that year. So, January 1, 1981 would be plotted at 1981.0. These rules apply regardless of the period of analysis selected. Labels on graphs showing four years or less on the horizontal axis provide month information, while those for longer periods simply show time in decimal years.

Selection of units of measurement for graphs and tables in EGRET

Data in the primary data frames of EGRET (`Sample` and `Daily`) and many of the data frames and matrices that store various summaries of results use SI units to store the data (there is one possible exception for discharge data in cases not involving water quality data analysis, this is described in section 'Discharge data from USGS data service'). The units for stored discharge values are m^3/s, for concentration they are mg/L, for flux they are kg/d, and for drainage area they are km^2. However, EGRET provides a high degree of flexibility for users to produce output in units that are more customary for the audience being addressed. They are also designed so that in most cases, careful selection of units can avoid having the output require the use of scientific notation (which makes graphs harder to read). The choices of output units are selected in the graph and table functions through the use

of an argument, which is `qUnit` for discharge and `fluxUnit` for flux. Figure 2 provides a list of the options available for `qUnit` and `fluxUnit`.

```
> printqUnitCheatSheet()
The following codes apply to the qUnit list:
1 =  cfs  ( Cubic Feet per Second )
2 =  cms  ( Cubic Meters per Second )
3 =  thousandCfs  ( Thousand Cubic Feet per Second )
4 =  thousandCms  ( Thousand Cubic Meters per Second )

> printFluxUnitCheatSheet()
The following codes apply to the fluxUnit list:
1 =  poundsDay  ( pounds/day )
2 =  tonsDay  ( tons/day )
3 =  kgDay  ( kg/day )
4 =  thousandKgDay  ( thousands of kg/day )
5 =  tonsYear  ( tons/year )
6 =  thousandTonsYear  ( thousands of tons/year )
7 =  millionTonsYear  ( millions of tons/year )
8 =  thousandKgYear  ( thousands of kg/year )
9 =  millionKgYear  ( millions of kg/year )
10 =  billionKgYear  ( billions of kg/year )
11 =  thousandTonsDay  ( thousands of tons/day )
12 =  millionKgDay  ( millions of kg/day )
```

Figure 2. Computer input and output showing the available choices of discharge units and flux units.

Users can always enter the command `printqUnitCheatSheet()` or `printFluxUnitCheatSheet()` to see these lists printed out. Within any function the units can be selected either by providing the code number or the name of the units. So, for example, if the user wanted to express discharge in thousands of ft^3/s, this could be done either by specifying `qUnit=3` or `qUnit=thousandCfs` as the argument to the relevant graphic or table function. Default units are always specified for any of these functions.

Flow History Analysis

Introduction

The purpose of this aspect of EGRET is to provide a very simple description of long-term variability and trend in discharge at a given streamgage. There are many factors that influence the year-to-year variations in discharge. These include changes in consumption of water or diversions of water into or out of the watershed, changes in groundwater storage in the watershed which influence base flow or storm flow, construction and operations of dams and levees, changes in land use patterns and land use practices (irrigation, urbanization, subsurface drainage, wetland drainage, or changes from deep-rooted natural vegetation to shallow-rooted agricultural crops), climate variability (phenomena such as El Niño, Pacific Decadal Oscillation, or Atlantic Multidecadal Oscillation), or long-term non-stationarity of climate possibly due to changes in greenhouse gas and particulate concentrations in the atmosphere. The methods presented here are intended to help the hydrologist determine the nature of the changes or variations that may be taking place in a given watershed. This can be used to pose or test hypotheses about the possible causes of these changes. It can also be used to help engineers and planners understand changing flow conditions that may be crucial to design or planning (flood protection measures, wastewater permits, or water availability for off-stream or in-stream uses). These analyses need to consider many different aspects of the discharge record. They may be focused on average discharges, low flows, or high flows. They may also be focused on a full annual perspective, or may be focused on one particular season. Seasonal analyses could be important for certain types of questions. One example could be a concern about the warming in winter months and determining what influence that might have on winter discharge in watersheds which have historically had large snowpacks and winter temperatures well below freezing. Another example would be a concern about decreasing

summer time minimum streamflow in a watershed where groundwater storage has significantly declined, potentially diminishing base flow to streams.

Flow history analysis in EGRET uses the daily discharge record for a given streamgage, organizes it according to some PA (such as water year or winter season) and then evaluates for the PA, for every year in the period of record, a set of statistics: The minimum 1 day mean daily discharge, the minimum 7-day mean daily discharge, the minimum 30-day mean daily discharge, the median of the mean daily discharges, the mean of the mean daily discharges, the maximum 30-day mean daily discharge, the maximum 7-day mean daily discharge, and the maximum 1-day mean daily discharge. Then, having computed those annual time series of these eight statistics it also produces a smoothed version of those time series, which emphasizes the broad multi-year variations and changes in the central tendencies of these time series.

With one exception (described below), the discharge statistics computed are all annual values (one value per year) where the year is as defined by the `paStart` and `paLong` parameters. That is, the period over which the statistic is computed starts with the first day of the month designated by `paStart` and runs through all the days in all of the `paLong` months of the Period of Analysis. So, for example if `paStart` is 12 and `paLong` is 4, the annual values of the statistic will be computed over the period from December 1 through March 31 and that statistic will be associated with the calendar year in which the period ends (the year containing the March 31 date that forms the end of the period). The one exception is the water year (`paStart=10, paLong=12`). In this case, all of the low flow statistics (1-day minimum, 7-day minimum, and 30-day minimum) are computed for the "climate year" which runs from April 1 through March 31. The use of the climate year for low-flow statistics (rather than the water year) is a common practice in hydrology, because it minimizes the probability that individual drought events will span multiple water years, which are by convention bounded by months that are typically

low flow months, and thus be counted twice in the same time series(Riggs, 1982; Gordon and others, 1991).

The smoothing method used in flow history analyses

The analysis of long-term variation in discharge characteristics used in this study builds on time-series smoothing methods that were pioneered by Cleveland (1979) and Cleveland and Devlin (1988). It is designed for analysis of long records (e.g. greater than 50 years duration, although it will work for shorter records) and it performs smoothing on annual statistics relevant to annual low flow, high flow, or annual mean flow. For this discussion define the discharge for year i as Q_i where that discharge can be any one of the eight streamflow statistics named in the preceding section (such a 7-day minimum, mean, or 1-day maximum) for the PA. For any given year i and discharge (Q_i) there is an associated time value (T_i), which is expressed in decimal years, as described in the section "Setting the period of analysis for graphs, tables, and analyses in EGRET". Thus, for any given flow statistic and PA there is a set of n values of Q_i and T_i, which constitute the time series to be smoothed.

The smoothing method used is based on locally weighted scatterplot smoothing (lowess) but with some particular features that are described below. The purpose of producing the smooth curves is to extract patterns of change that describe variations at time spans of about a decade or more. Such curves are very resistant to the influence of one or two years with extremely high or low flows. They will also tend to smooth out changes that are actually very abrupt, for example those that come about because of construction or removal of a dam or initiation of a major new water diversion.

The variable y_i is the log-transformed value of the flow statistic:

$$y_i = \ln(Q_i), \tag{1}$$

The logarithm transformation is applied because discharge data typically are highly skewed, approximating a log-normal distribution in many cases. Using the logarithm transformation results in weighted regressions in which the residuals are more nearly normal and thus, individual extreme values do not exert a large amount of influence on the estimates. This results in a more robust smoothing process. It also means that the smoothed values, denoted $\hat{Q}_i$, are more nearly an approximation of the median of the time series than they are an approximation of the mean (see Helsel and Hirsch (2002), pages 254-260 for a discussion of transformation issues).

In log-space, the smooth curve is defined by a series of n-weighted regressions on the data set. The estimate, $\hat{y}_i$, of y_i is defined as

$$\hat{y}_i = \beta_{0i} + \beta_{1i} \bullet T_i \quad \text{for } i = 1, \text{n} \tag{2}$$

where β_{0i} is the estimated regression intercept for the regression model fitted for year i, and β_{1i} is the estimated regression slope for the regression model fitted for year i.

The two regression coefficients, β_{0i} and β_{1i}, are computed from a weighted regression, where the weights are equal to one for the observation for the year in which the estimate is being made, and decay to zero at a time separation of 30 years between a given observation and the time of the estimate. Thirty years is the default value used for the weight function and is used in the discussion below, but the EGRET user can change this to a different value. The specific weights are computed with the Tukey tri-cubed weight function (Tukey, 1977). The weight for the i^{th} streamflow value in the computation of the smoothed value for the j^{th} year is:

$$w_{i,j} = \begin{cases} \left(1 - \left(d_{i,j}/30\right)^3\right)^3 & if \left|d_{i,j}\right| \le 30 \\ 0 & if \left|d_{i,j}\right| \ge 30 \end{cases} \tag{3}$$

where,

$$d_{i,j} = T_i - T_j \tag{4}$$

Figure 3 shows the shape of the weight function. The weight function sets a weight of zero for all observations that are more than 30 years from the central year (the year for which the estimate is being made). All of the values for the years that are between zero and 15 years before the central year have weights that are at least 67% as large as the largest weight. The largest weight is for the observation from the central year. The default "half-window width", 30 years, was selected by visual examination of graphics for many alternatives for many different discharge records. The half-window width was selected to be as narrow as possible, such that individual year-to-year oscillations are fully damped out. Although 30 years is the default value for the half-window width used in EGRET, it can be modified by the user, using the `window` argument in the function `setPA`.

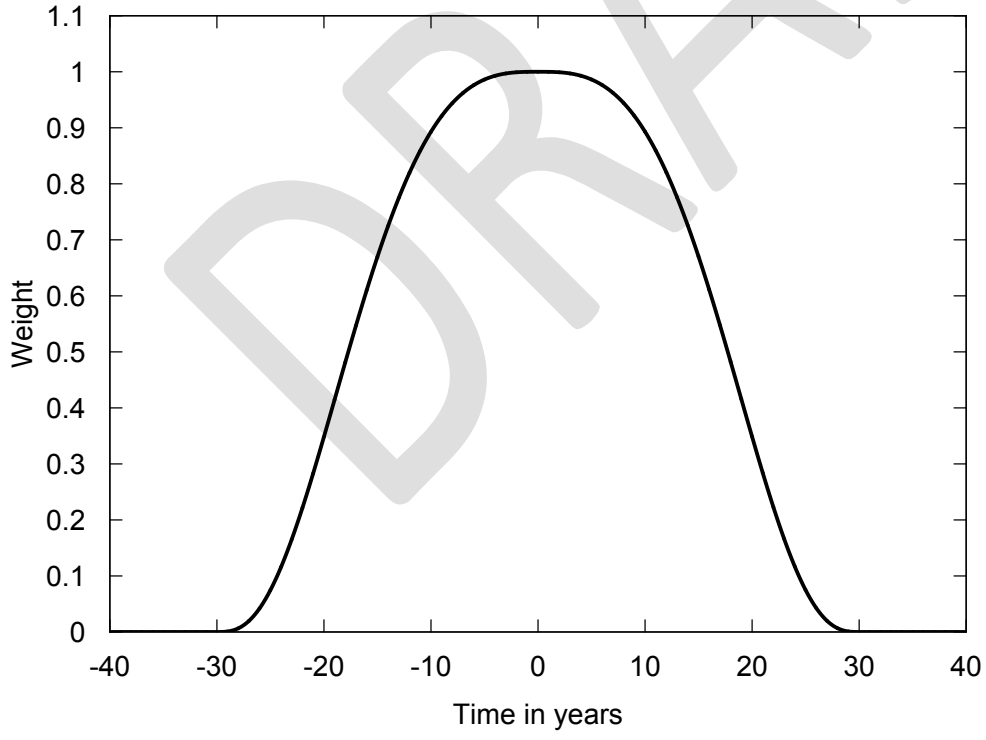


Figure 3: Values of the triCube weight function used in weighted regressions for smoothing discharge time series. Half-width is set to its default value of 30 years.

The final step in producing the graphic of the smoothed annual values is the retransformation:

$$\hat{Q}_i = \exp(\hat{y}_i) \tag{5}$$

This retransformation is designed to produce a smooth representation of the median of the distribution over time for the statistic being plotted.

The next section shows the EGRET commands needed to run this type of analysis and provides examples of graphical and tabular outputs available.

EGRET functions for flow history analysis

The set of steps needed to conduct the analyses described in the proceeding section are defined here. For completeness, these will include the data retrieval steps which are described more fully in the data retrieval section of the report. This example will consider the discharge record for the Spokane River at Spokane, WA USGS streamgage 12422500. This particular record was chosen because it is very long (starting 1891-04-01) and is complete to the present and because it is a discharge record that has shown substantial change, particularly in terms of declining low-flow conditions, due to a long history of depletion of water from the Spokane Valley - Rathdrum Prairie Aquifer. This set of commands is shown here with explanation of the purpose of that command immediately after it.

```
sta <- "12422500"
```

This specifies that the streamgage of interest is USGS number 12422500.

```
param <- "00060"
```

This specifies that the parameter of interest is daily discharge (00060).

```
Daily <- getDVData(sta, param, StartDate = "", EndDate = "")
```

This retrieves the discharge data set from USGS data services and forms it into the Daily data frame, which includes daily discharge as well as 7-day and 30-day average discharge for each date in the record.

```
INFO <- getMetaData(sta, param)
```

This initiates an interactive process of retrieving the meta-data for the site and parameter. It provides some of that information back to the user and prompts the user for various types of text information for labeling of files and graphics. All of the metadata, including the user responses to prompts are stored in the `INFO` data frame.

The function `setPA`

This function is required for setting up the Period of Analysis and window width to be used in the analysis. In the default case the function sets up the period of analysis as the water year and sets the half-window width to 30 years. The function performs no computations but simply augments the meta-data stored in the `INFO` data frame with the `paStart`, `paLong`, and `window` values. In the default case the command is simply:

```
INFO <- setPA()
```

If the user is selecting other values, say a PA that covers the months December through February and a half window width of 20 years, the call would be:

```
INFO <- setPA(paStart = 12, paLong = 3, window = 20)
```

The function `makeAnnualSeries`

This function creates a matrix called `annualSeries` to store the annual series of discharge statistics. It computes and stores those statistic values in `annualSeries`, and then computes the smoothed estimates of these statistics and stores them in `annualSeries`. The command is:

```
annualSeries <- makeAnnualSeries()
```

The dimensions of `annualSeries` are (3,8,n) where n represents the number of years for which one or more of the annual discharge statistics can be calculated. In the Spokane River example shown above `annualSeries` has dimensions (3,8,124). For the first dimension: 1 is for storing the mean value of `decYear`, the decimal time value, for all of the daily discharge values used to compute the statistic of interest; 2 is the actual discharge statistic for that particular year; and 3 is the smoothed value of that discharge statistic for that particular year. The second dimension is the index of the discharge statistic. The index of these discharge statistics is known as `istat`. The `istat` values for the eight discharge statistics are defined in Table 5.

Table 5. Definitions of the eight discharge statistics computed in EGRET

istat	statistic name
1	annual 1-day minimum flow
2	annual 7-day minimum flow
3	annual 30-day minimum flow
4	annual median flow
5	annual mean flow
6	annual 30-day maximum flow
7	annual 7-day maximum flow
8	annual 1-day maximum flow

The third dimension of the `annualSeries` matrix is an index of years, from 1 through n. There can be NA values for some of these statistics if the amount of data available for computing the statistic is less than 90 percent of the number of days that would exist in a complete record for that period. Thus the first year that will have a value will be the first year in which the data set for the PA is 90 percent or more complete, and similarly the last year that will have a value will be the last year in which the data set for the PA is 90 percent or more complete. For example, for a water year or calendar year there must be more than 328 days of available data in order for the statistic to be computed for that year. Note that because of the way that the 7-day or 30-day statistics (`istat` = 2, 3, 6, and 7) are computed,

the set of days that define the annual discharge statistic can sometimes be centered on a date which slightly precedes the specified PA of the specified year.

In the example shown here, the annual 7-day minimum flow for the first year of the record would be stored as `annualSeries[2,2,1]`. Its smoothed value would be stored as `annualSeries[3,2,1]`. The mean decimal year value for the dates used to compute this discharge statistic would be stored as `annualSeries[1,2,1]`.

Plotting the results for a single discharge statistic using `plotFlowSingle`

The actual values of a given discharge statistic and their smoothed values can be plotted using the function `plotFlowSingle`. The specific discharge statistic (`istat`) must be specified in the call to this function. There are many other arguments that can be specified (see `?plotFlowSingle` or Appendix B), the only one that will be mentioned here is the selection of discharge units to be used. Discharge units are specified by the argument `qUnit`. In this example the units of m^3/s are specified, (`qUnit = 2`). The default is `qUnit = 1` (which is ft^3/s). The function call for annual 7-day minimum discharge, in units of m^3/s is:

```
plotFlowSingle(istat = 2, qUnit = 2)
```

The resulting graphic is shown in Figure 4.

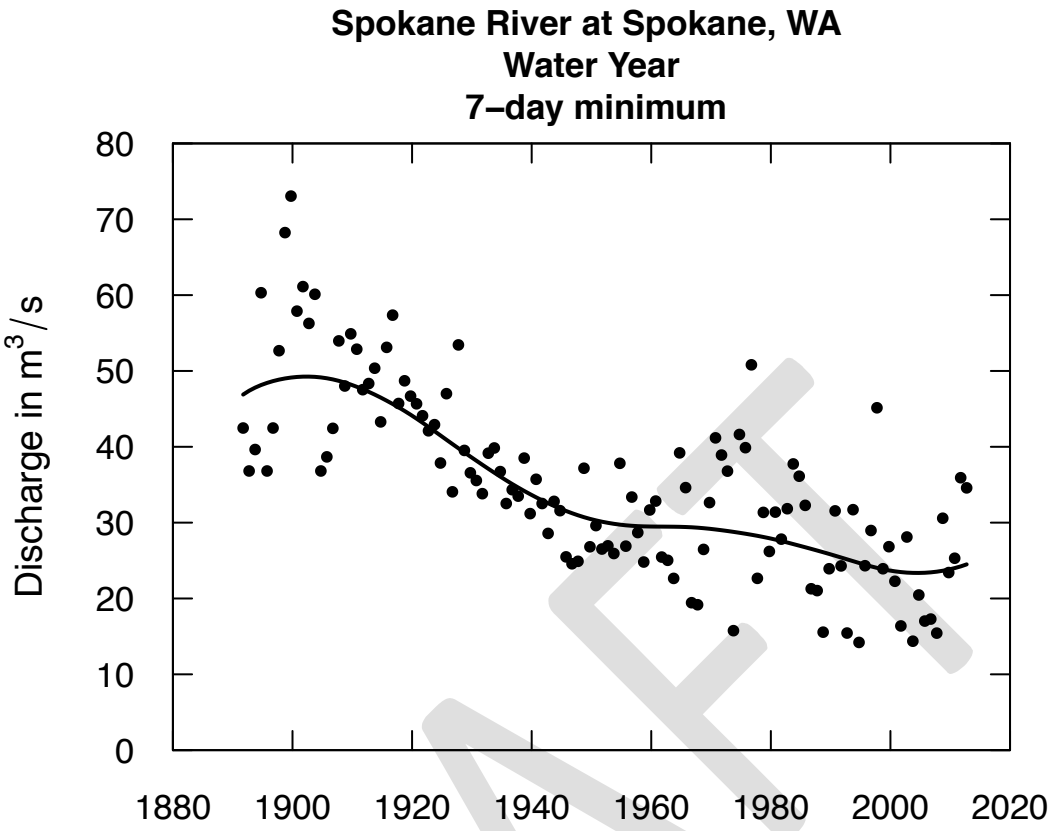


Figure 4. Plot of the 7-day minimum discharge by year (dots) and smoothed estimates (curve).

Printing out results for a single discharge statistic using `printSeries` and `tableFlowChange`

To generate a table suitable for printing or for input to some other analysis, the values displayed in the output from `plotFlowSingle` can be produced with the function `printSeries`. The only argument that must be specified for this function is `istat`, all others can be their default values. Producing a table of numbers that corresponds to Figure 4 but with the discharge values reported as runoff in mm/day, can be done with the following command:

```
SpokaneSeries <- printSeries(istat = 2, runoff = TRUE)
```

This command does two things, it creates a data frame, in this case called `SpokaneSeries` that contains the tabular information, and it also prints the information to the console. The printed output is shown in Figure 5. By creating the data frame called `SpokaneSeries` in this example, these results can

```
Spokane River at Spokane, WA
 Water Year
    7-day minimum
    runoff in mm/day
   year   annual   smoothed
           value    value

   1892    0.330    0.365
   1893    0.286    0.369
   1894    0.308    0.372
   1895    0.469    0.374
   1896    0.286    0.377
   1897    0.330    0.378
   1898    0.410    0.380
......... output edited ....
   2003    0.219    0.182
   2004    0.112    0.182
   2005    0.159    0.182
   2006    0.132    0.182
   2007    0.134    0.182
   2008    0.120    0.183
   2009    0.238    0.184
   2010    0.182    0.185
   2011    0.197    0.187
   2012    0.279    0.188
   2013    0.269    0.190
```

Figure 5. Output of the annual 7-day minimum discharge and smoothed values of annual 7-day minimum discharge in mm/day.

be written to a file, which can then be used as input to some other computer application including input to a spreadsheet or word processing application for use in producing a table suitable for publication. Details on how to make such conversions are provided in Appendix A, section 6. In addition, the results shown in Figure 4 can also be expressed in terms of the amount of change estimated to have taken place between any two years in the smoothed time series. This can be done with the function `tableFlowChange`. The function describes these changes between selected pairs of years in four

different ways. For a comparison between two times, T_i and T_j (expressed in decimal years), where the smoothed values of discharge at those times are denoted $\hat{Q}_i$ and $\hat{Q}_j$ `tableFlowChange` will express the change as:

- A change between the first and last year of the pair, expressed in the flow units selected. $\hat{Q}_j - \hat{Q}_i$
- A change between the first and last year of the pair, expressed as a percentage of the value in the first year. $\left(\hat{Q}_j - \hat{Q}_i\right) \bullet 100 / \hat{Q}_i$
- A slope between the first and last year of the pair, expressed in terms of the flow units per year. $\left(\hat{Q}_j - \hat{Q}_i\right) / (T_j - T_i)$
- A slope between the first and last year of the pair, expressed as a percentage change per year (a percentage based on the value in the first year). $\left(\hat{Q}_j - \hat{Q}_i\right) \bullet 100 / (\hat{Q}_i \bullet (T_j - T_i))$

There are four arguments that are needed by `tableFlowChange`. The first is `istat` that determines which flow statistic is being analyzed. This argument has been introduced earlier, and it has 8 possible values, which are listed in Table 5. The second is `qUnit`. The default value is `qUnit` = 1, which corresponds to ft^3/s, but all four options for qUnit values listed in Figure 2 are possible. The third is `runoff`, for which the default value is `FALSE`. If `runoff` is `TRUE` then the results are provided in units of mm/day. The final argument is called `yearPoints`. The object `yearPoints` is a vector of integer numbers that represents the full set of years for which the user wants to make comparisons. This is best explained by an example. If one wanted to examine the changes in discharge from 1950 to 1980 and 1980 to 2010, then `yearPoints` would be specified as:

```
yearPoints <- c(1950, 1980, 2010)
```

That indicates that the full set of comparisons (changes or slopes) that will be made are all possible ordered pairs of these years, which is 1950-1980, 1950-2010, and 1980-2010. In the example

of the Spokane River 7-day minimum flow example, one might choose comparisons in blocks of 40 years each. The commands would be:

```
yearPoints <- c(1892,1932,1972,2012)
tableFlowChange(istat = 2, qUnit = 2, yearPoints=yearPoints)
```

or it could be done in a single command line as:

```
tableFlowChange(istat = 2, qUnit = 2, yearPoints = c(1892,1932,1972,2012))
```

The output is shown in **Error! Reference source not found.**:

```
  Spokane River at Spokane, WA
  Water Year
   7-day minimum

             Streamflow Trends
  time span          change        slope       change        slope
                       cms        cms/yr          %           %/yr
1892  to  1932          -10        -0.26          -22        -0.54
1892  to  1972          -18        -0.23          -39        -0.49
1892  to  2012          -23        -0.19          -48         -0.4
1932  to  1972         -8.2        -0.21          -22        -0.55
1932  to  2012          -13        -0.16          -34        -0.42
1972  to  2012         -4.4        -0.11          -15        -0.38
```

Figure 6. Output from tableFlowChange.

Plot changes in variability with `plotSDLogQ`

This graphic is designed to indicate if there are changes taking place in the overall variability of the daily discharge record, without regard to the question of whether the central tendency is changing over time. The function `plotSDLogQ` produces a graphic of the running standard deviation of the log of mean daily discharge. By using the standard deviation of the log discharge the statistic is dimensionless. It is a measure of relative variability. If, for example, the probability distribution of mean daily streamflows were to have trended upwards (or downwards) over time, but done so in a manner that all quantiles of the distribution had increased by the same percentage amount, then we

would expect this graphic to show a horizontal line. If, on the other hand, the change in the probability distribution was such that there was a greater percentage change in the high end and/or low end of the distribution, as compared to the percentage change in the middle portion of the distribution, then this curve would slope upwards over time. It is much like a graph of a moving coefficient of variation, but it has sample properties that make it a smoother measure of the changing variability in the data. This graph can be useful in providing empirical evidence regarding hypotheses regarding the idea that increasing urbanization or increasing greenhouse gas concentrations in the atmosphere are bringing about changes in hydrologic variability. This is just one simple way to explore such questions. The function can be called with the command:

```
plotSDLogQ()
```

The computation is made using a moving window over which the standard deviation is computed. The default width of this window is 15 years. Users can select a different width using the argument window. So if the user wanted to use 20 years the command would be

```
plotSDLogQ(window = 20)
```

Assuming that the 15 year default window is used, the computations begin with a window centered on a date that is 7.5 years from the start of the record and computes the standard deviation of the natural logarithm of the mean daily discharges for all the days from 7.5 years before to 7.5 years after that center date and the result is what is plotted on the graph, for that center date. Note that the "window" argument to `plotSDLogQ` specifies a non-weighted rectangular window over which to compute the standard deviation, in contrast to the "window" argument to `setPA`, which specifies a weighted smoothing window for computing other statistics. The computation then moves on to a new center date that is a tenth of a year later (36.5 days later) and repeats as many times as necessary until it reaches a center date that is 7.5 years before the end of the record. The user can limit the span of the calculation with the use of two arguments, `yearStart` and `yearEnd`, expressed in decimal calendar

years. The defaults for these are the start and end of the available record in the `Daily` data frame. For an example of this plot (Figure 7), the data set used is the discharge record from the Colorado River at Lees Ferry, Arizona. This case is an interesting one because it shows such a strong trend towards decreasing variability, a result of the history of increasing water management through reservoir storage, diminishing the size of the highest discharges and increasing the size of the lowest discharges.

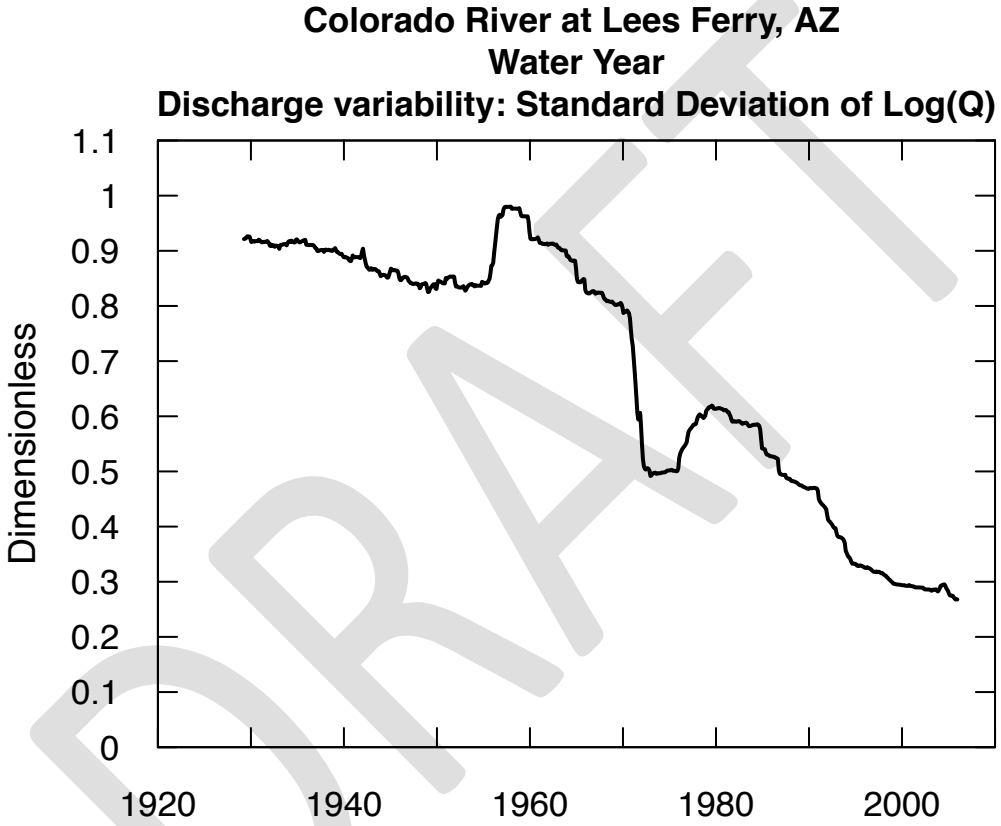


Figure 7. Graph of the standard deviation of Log(Q) over time, Colorado River at Lees Ferry, AZ.

If the user is interested in changes in variability in a particular season, the desired PA can be specified prior to running, `plotSDLogQ` by using the `setPA` function. For example, to consider variability in the months of June, July, and August the commands would be:

```
INFO <- setPA(paStart = 6, paLong = 3)
plotSDLogQ()
```

The resulting graph will be appropriately labeled to indicate the PA used.

Graphics for plotting the discharge record, `plotQTimeDaily`

Plotting the complete discharge record is a common task and the function `plotQTimeDaily` makes that possible. It can be called with all of its arguments set to their default values and will produce a suitable graphic. Figure 8 presents an example of such a plot for the Big Sioux River at Akron, IA for 1941-2011. The command in this case was:

```
plotQTimeDaily(lwd = 1,qUnit = 2)
```

The specific arguments called are `lwd = 1` for setting the line width narrower than the default (which is `lwd = 3)` and `qUnit = 2` (to select m^3/s as the units for the graph). The color red is the default. This is done to prevent segments of the discharge record from being confused with the black tick marks.

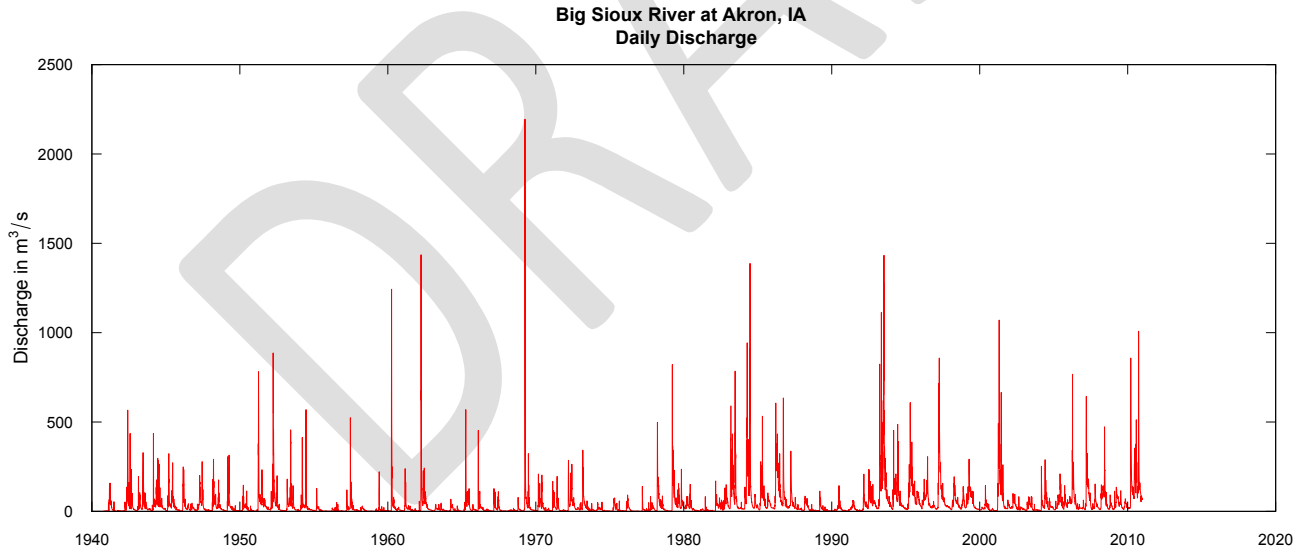


Figure 8. Graph of daily discharge record for the Big Sioux RIver at Akron, IA

Another use for this function is to plot only those periods in which discharge is higher than some threshold value. This can be useful in discussions that relate to possible changes in the magnitude and/or frequency of high discharge events. Using the same record, with a threshold of 600 m^3/s, this could be accomplished with the command `plotQTimeDaily(qLower = 600, lwd = 3)`. The resulting graph is shown in Figure 9:

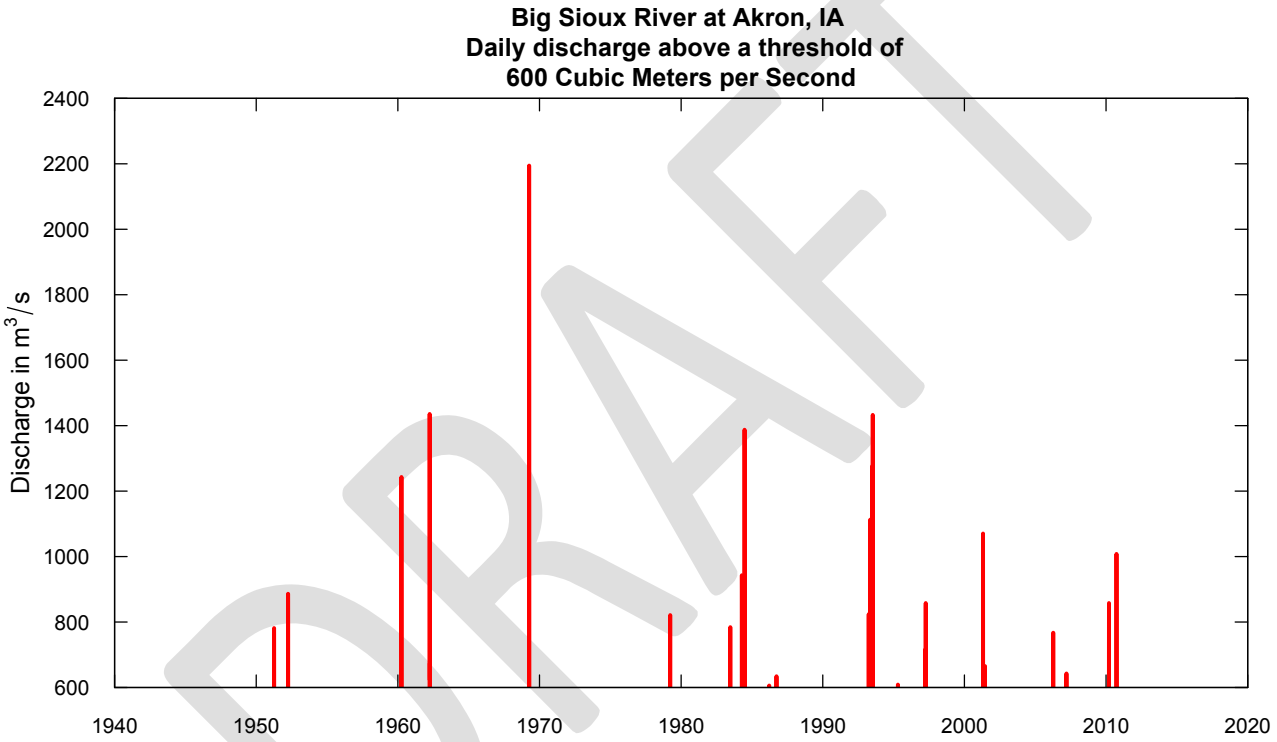


Figure 9. Output from `plotQTimeDaily` for Discharge data for Big Sioux River at Akron Iowa, showing discharges only above 600 m^3/s.

A graphic of this type can be useful in the magnitude and frequency of high discharge events. It can be very helpful in illustrating the persistence in high discharge events (the tendency for high flows

to occur in groups rather than a random pattern) and also reveal patterns of changing magnitude and/or frequency of high discharge.

Multipanel graphics for flow history

There are three specific multipanel graphics functions for depicting discharge history information. One of these is `plotFour`. It is a combination of three panels produced by `plotFlowSingle` and one panel produced by `plotSDLogQ`. The three panels from `plotFlowSingle` are those for the 1-day maximum, the mean, and the 7-day minimum. These can be done for any PA, depending on the questions of interest. Although the component graphic functions that make up the four panels of this plot (plotFlowSingle and plotSDLogQ) each allow the user to set a maximum value for the vertical axis, this function and others similar to it, set these automatically so that the scales for each panel extend to a value slightly larger than the maximum value in the specific data set being plotted in that panel. Users should recognize that the annual 1-day maximum is not the same as the annual peak discharge. The annual peak discharge is intended to represent an instantaneous maximum discharge value for the year. The 1-day maximum will always be a smaller value. On large rivers, where discharge changes slowly, there may be very little difference between the 1-day maximum and the annual peak, and they will typically be very highly correlated with each other. On small streams where discharge can rise in the course of a single day from very low flow value to an annual maximum within a single day, there can be very large differences between these values and the correlation between the two time series may be very low.

Figure 10 is an example for the Big Sioux River

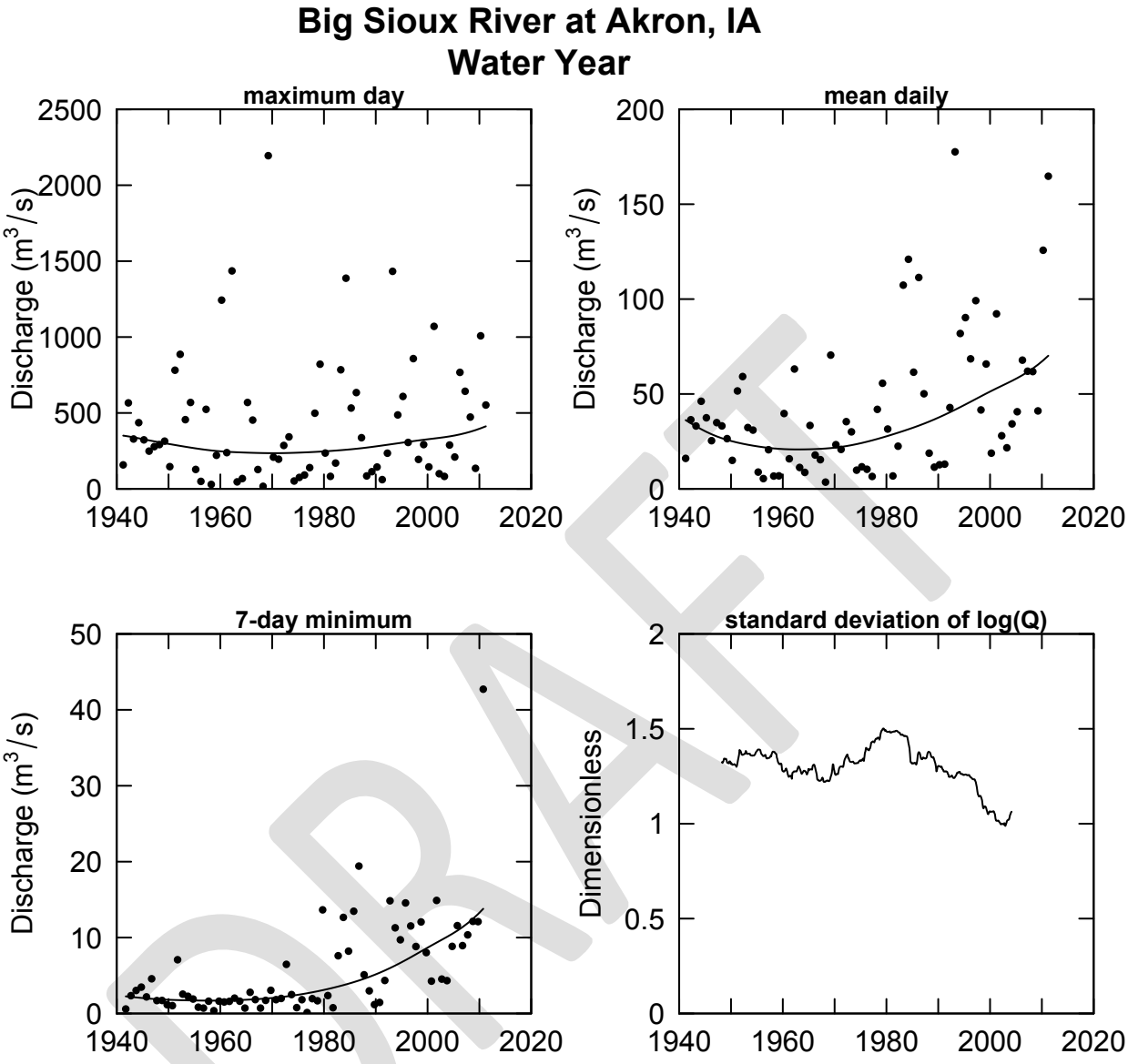


Figure 10. Example of graphics produced by `plotFour` function.

This type of graphic can be particularly useful in exploring changes that may be focused on one particular part of the year. The following example is for the very long discharge record of the Merced River at Happy Isles Bridge, which is located high in the Sierra Nevada Mountains in Yosemite National Park, California. The warming conditions of the past several decades are having an impact on

wintertime flow conditions and this is illustrated with this example where the PA is the two months January and February. The commands needed to produce Figure 11 were this combination (after the `Daily` and `INFO` data frames had been created).

```
INFO <- setPA(paStart = 1, paLong = 2)
annualSeries <- makeAnnualSeries()
plotFour(qUnit = 2)
```

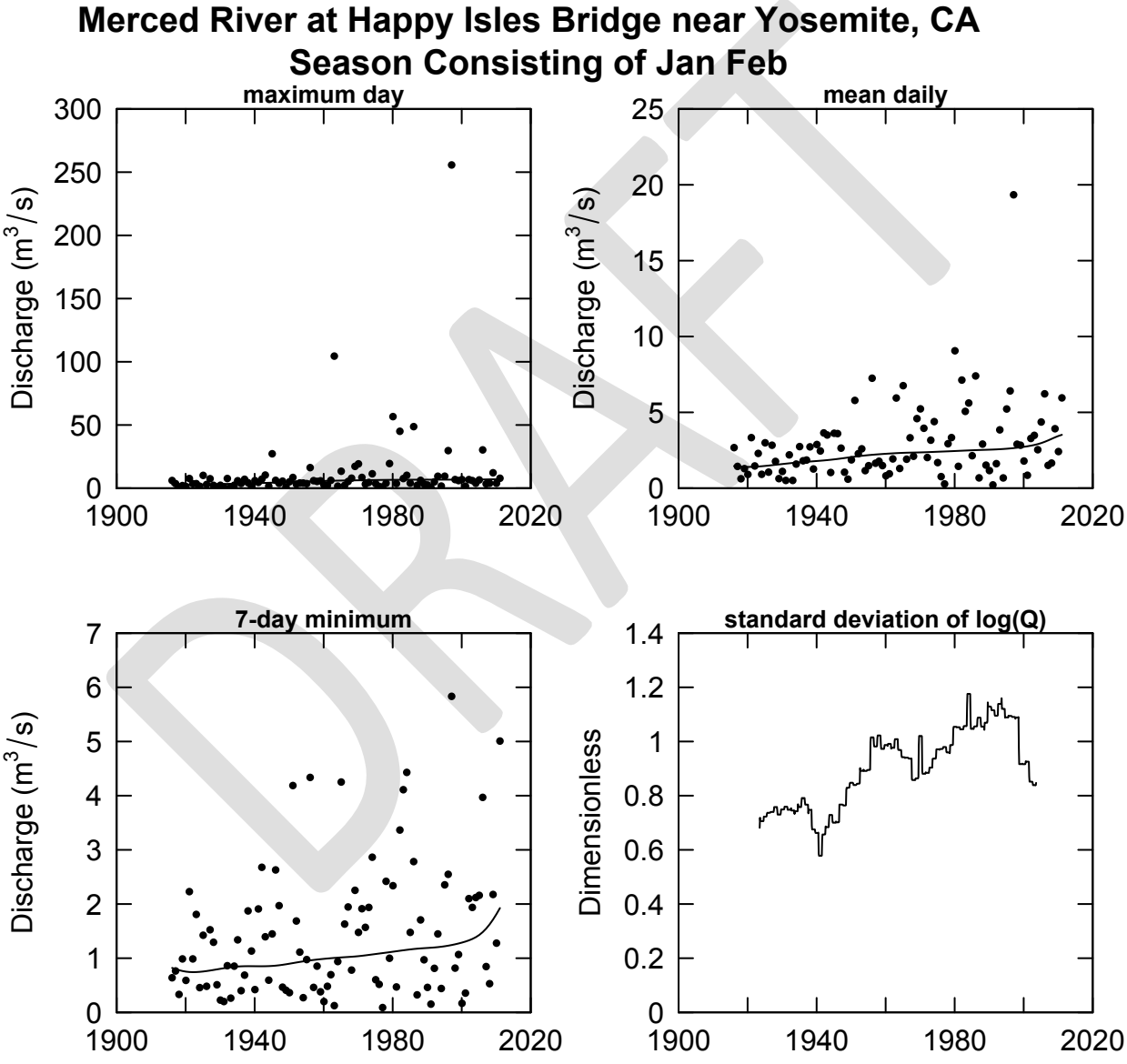
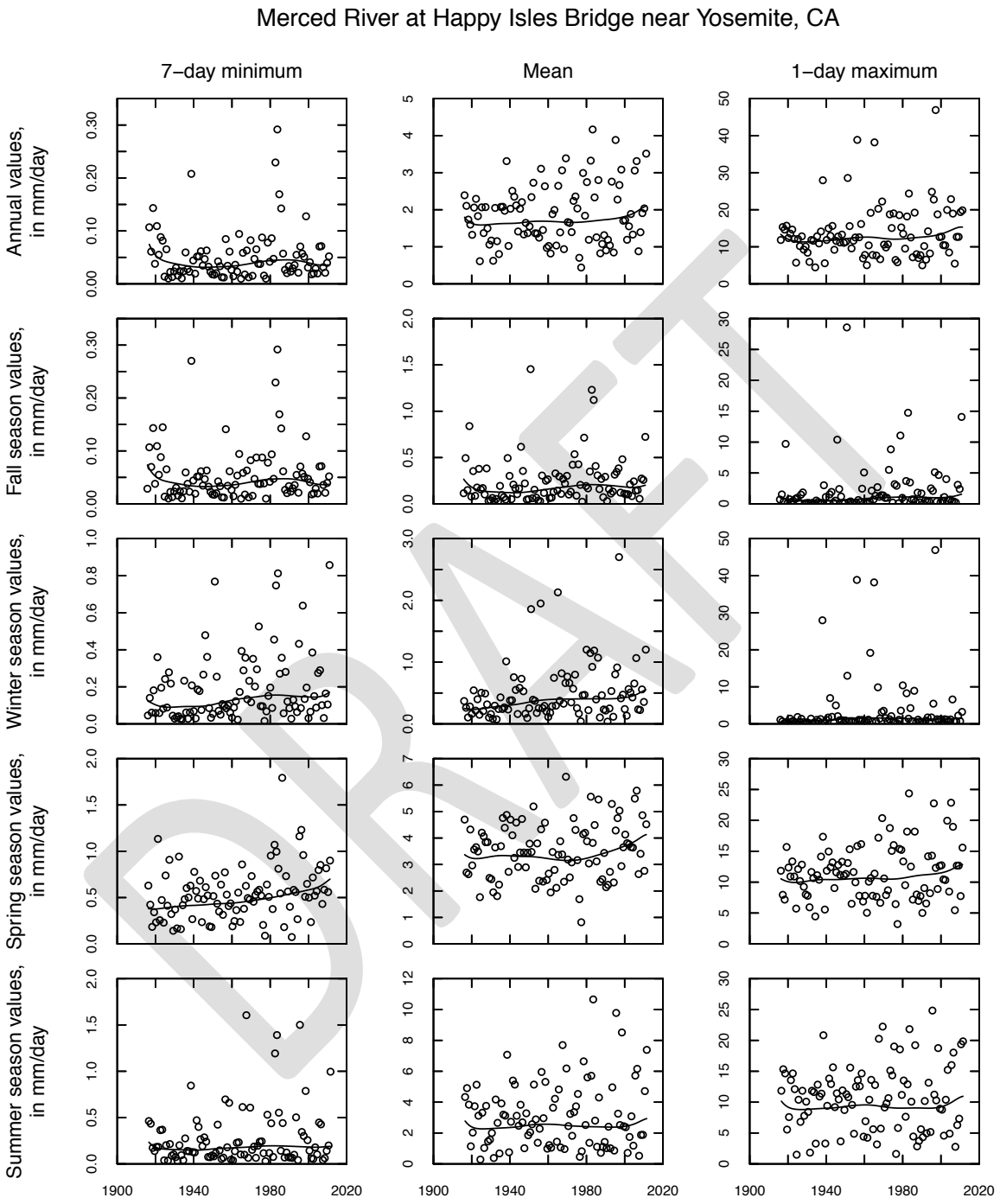


Figure 11. Output from `plotFour` for the Merced River.

The next function `plotFourStats` is nearly identical to `plotFour`, the only difference being that the standard deviation of log(Q) is not part of it, but it is replaced by the median discharge. The reason for having such a similar function available is that the standard deviation of log(Q) is somewhat unconventional and some users may find it difficult to explain to their audience, `plotFourStats` provides a more conventional alternative. Users who have some knowledge of R programing can easily adapt these functions to plot other combinations of the statistics calculated. This can be done by selecting different values of `istat` into the calls to `plotFlowSingle` that are included in the code for `plotFour`. Finally, there is the much more elaborate graphic, `plot15`. It produces a set of 15 plots (all based on `plotFlowSingle`). They include the 1-day maximum, mean, and 7-day minimum for 5 different PAs. These PAs are the water year, Fall (September, October, November), Winter (December, January February), Spring (March, April, May) and Summer (June, July, August). Because of its complexity and detail this figure is best produced as output to a file, but it can be plotted to the computer screen. Before plotting it to the computer screen the user should set up a graphics window first to accommodate it (a window with a height that is greater than its width). The commands for producing it as a pdf are:

```
pdf("plot15.pdf",height=10,width=8)
plot15(yearStart=1900,yearEnd=2012)
dev.off()
```

Figure 12 shows the results of these commands for the Merced River discharge data set.



Streamflow statistics (circles) in units of millimeters per day, annual values and seasonal values
Fall (Sept., Oct., and Nov.), Winter (Dec., Jan., and Feb.), Spring (Mar., Apr., and May), and Summer (June, July, and Aug.)
and locally weighted scatterplot smooth (solid curve) for Merced River at Happy Isles Bridge near Yosemite, CA for 1900 – 2012.

Figure 12. Output from `plot15`, Merced River at Happy Isles Bridge near Yosemite, CA.

This graphic can be used to provide a quick overview of changes in streamflow for a large number of rivers within a region. An example of its use in that manner is found in the Appendix to Rice and Hirsch (2012).

Summarizing Water Quality Data (without using WRTDS)

The EGRET software includes several functions that produce summary information about water-quality data and the associated discharge data. First, they provide a quick means of identifying problems with the data set by showing observations that seem highly unusual and should be investigated before proceeding with the analysis. If these values can be shown to be clearly in error they should be deleted or edited so that they are correct. If they appear to be correct, but are highly unusual their influence on the results of subsequent analysis should be evaluated. Steps that can be taken to remove or edit an observation in the data set and also to explore sensitivity to extreme observations is discussed in the section "Editing data sets". The summary information can also provide insight on important properties of the data set. For example it might reveal the nature of the relationship between concentration and discharge, the presence and nature of seasonality in the data, or the presence of gradual or abrupt trends in the data. It may also show temporal patterns in the data collection such as long gaps in the record, changes in the frequency of sampling, or very limited sampling in certain seasons. The existence of long gaps (more than about 2 years) can be important to the interpretation of WRTDS results, and a specific function (`blankTime`) is provided to deal with the issues of long data gaps. In cases where there is little or no sampling in certain seasons (most commonly the winter season), the user may want to restrict the WRTDS results that are presented by setting the PA to the sampled months (for example confine the results to April through November using `paStart = 4`,

paLong = 8). Also, changes in laboratory reporting practices may be revealed, such as shifts in censored data reporting levels or changes in rounding practices (e.g. for some period of time values are reported as 0.1, 0.2, 0.3, …. but in later years they are reported with many more significant figures such as 0.137, 0.218, 0.307). When this happens the user may want to consider these more rounded values to be interval censored (so that 0.1 might be represented as a range of 0.05 to 0.015). The section "Editing data sets" provides suggestions for doing this type of data recoding.

The types of plots presented here may be highly useful in confirming various types of findings in the WRTDS results. Many audiences, including the data analyst, may view the rather complex smoothing approach used in WRTDS with skepticism. Confirmation of findings using much simpler graphical means can provide useful confirmation of the WRTDS inferences and suggest further analysis that should be considered.

The following sections describe and show examples of these functions. They are shown here with most arguments at their default levels and only a few crucial arguments used. The graphic functions described in this section all have the ability to produce plots for data from all times of year or to produce plots that are restricted to a specific PA (see section above "Setting the period of analysis for graphs tables, and analyses in EGRET"). Restricting the graphics to a particular PA is accomplished by using the setPA function. If, for example, we wanted a graphic specific to the months December, January and February, the command INFO <- setPA(paStart=12, paLong=3) would be given prior to the specific plotting command. The graphic resulting from that plotting command will state what months are included. If a previous plot used a PA that was not 12 months in length and the next plot was intended to cover the full year then the command INFO <- setPA() must be used to reset the PA to the water year (because the defaults for setPA include paStart=10 and paLong=12). For fuller descriptions of all of the flexibility of these functions users should refer to Appendix B.

plotConcTime

This function produces a time series graph of the constituent concentration values as a function of time. In its simplest form the command is:

```
plotConcTime()
```

This will produce a graphic of all of the concentration values versus time for the entire period of record (every row of the `Sample` data frame). The convention for showing a censored value is the use of a line segment rather than a simple point for these observations. Table 6 lists the important arguments for this function that can be used to modify the y-axis scale or cause the plot to cover a selected subset of the full data set.

Table 6. Important arguments for the function `plotConcTime`

Arguments	Purpose and options	Default
`logScale`	If TRUE, plots concentrations on a log scale. If FALSE, plots concentration on an arithmetic scale, with minimum = 0.	`logScale = FALSE`
`concMax`	Specifies a maximum value for the vertical scale, a concentration in mg/L. The default allows it to be set automatically based on the data. The `concMax` argument can be used to standardize a set of graphics through a given report.	`concMax = NA`
`concMin`	Only used when `logScale=TRUE`. Sets the minimum value on the vertical axis. Must be > 0. It is a concentration in mg/L.	`concMin=NA`
`qLower`	Sets a lower bound on the discharge values for the set of sample values shown in the figure. It is expressed in the discharge units selected by user. See `qUnit` argument below.	`qLower = NA` (this is equivalent to a lower bound of zero)
`qUpper`	Sets an upper bound on the discharge values for the set of sample values shown in the figure. It is expressed in the discharge units selected by the user.	`qUpper = NA` (this is equivalent to having no upper bound)
`qUnit`	Selects the units for discharge values used in qLower and qUpper.	`qUnit = 2, which is` m^3/s

To understand the way that the various features of this function can be used, we will consider the case of nitrate trends in the Choptank River on the eastern shore of Chesapeake Bay. This is a highly agricultural watershed, with highly permeable soils and shallow aquifers. Increasing concentrations of nitrate in groundwater over the past few decades have been documented in this region (Debrewer, and others, 2008). The question to be considered is what kinds of changes have taken place in nitrate in the

surface water of this area. The data set is very rich. It is, in fact, the type of data set for which WRTDS was designed. Figure 13 is the graphic produced by the command

```
plotConcTime().
```

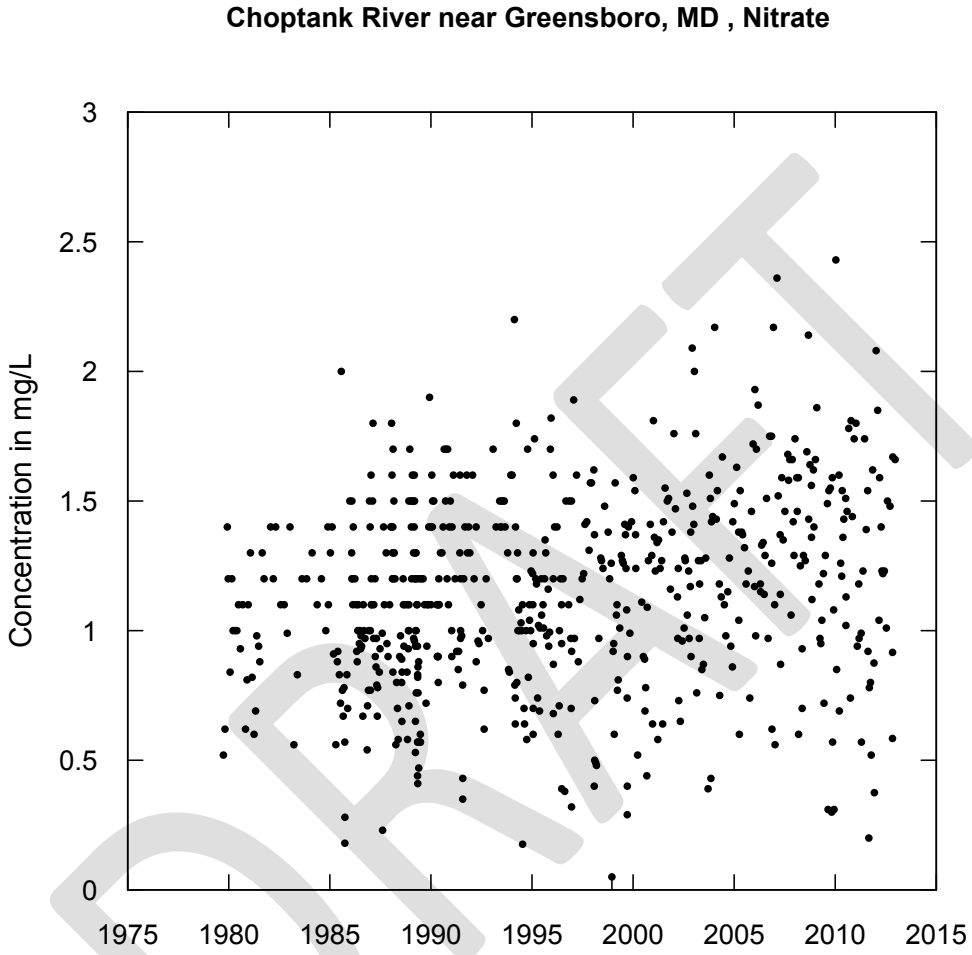


Figure 13. Concentration versus time, Choptank River near Greensboro Maryland, Nitrate.

The general idea that concentrations have trended upwards over the period from about 1980 to 2012 is clear at a glance. It is complicated by the change in reporting rules that caused the early years of the record to have the reported values that were greater than 1 mg/L to be rounded to the nearest tenth of a mg/L and after about 1996 this rounding was eliminated. The `plotConcTime` function allows for more specific exploration of the nature of changes in this system. For example, there may be a strong

interest in conditions in a particular part of the year and the changes that are taking place at different discharge conditions. One can isolate a season, in this case the months of April, May and June, by setting the PA using the setPA function. Figure 14 shows the results from the two commands

```
INFO <- setPA(paStart = 4, paLong = 3)
plotConcTime()
```

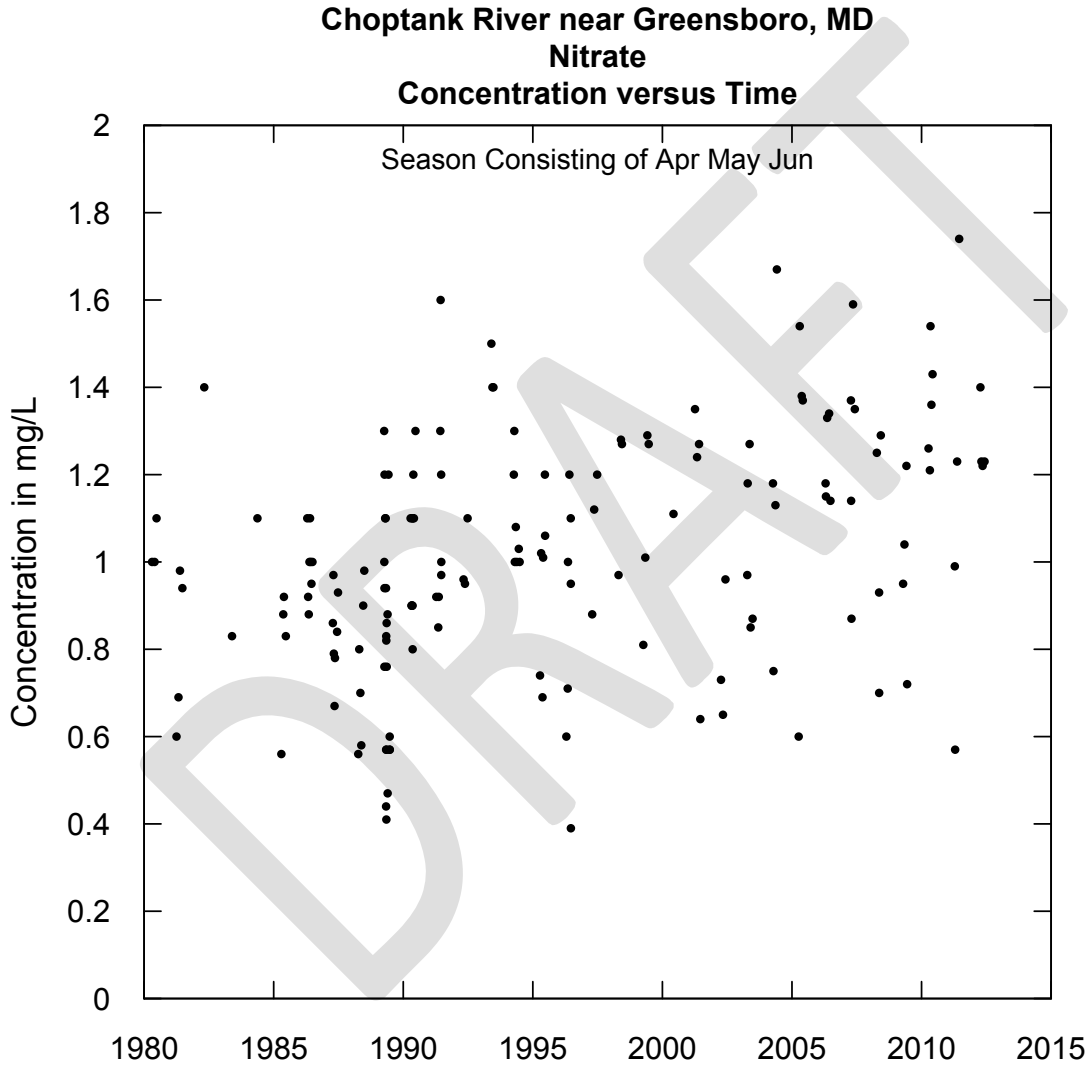


Figure 14. Concentration versus time, Choptank River near Greensboro, Maryland, Nitrate, for April, May and June

The upward trend continues to be evident when only this season is considered. But, it may also be of interest to know if the trend is specifically focused in a particular range of discharge values during this season. This can be done using the `qLower` and `qUpper` arguments. Using these arguments, `plotConcTime` will selectively plot only those concentrations that happened on days when the mean daily discharge was greater than `qLower`, or days when mean daily discharge was less than `qUpper`, or if both arguments are used, it would plot only those data collected on days with discharge in the range between `qLower` and `qUpper`. The values of `qLower` and `qUpper` are specified in units selected by the user and specified in the argument `qUnit`. If `qUnit` is not specified then the default is used (which is `qUnit = 2`, which causes the units to be m^3/s). The full set of options for `qUnit` is shown in Table 2. The following is an example of the use of this capability (it is assumed here that the PA has already been set by `setPA`, if in doubt the user can verify it by giving the command `INFO` or just using the `setPA` function again). The command used to produce the desired plot is:

```
plotConcTime(qUnit=1,qUpper=165,qLower=34)
```

specifies that the plot should show all the concentration data collected on days with discharge in the range of 34 to 165 ft^3/s during the three month period starting in April. The results are shown in Figure 15.

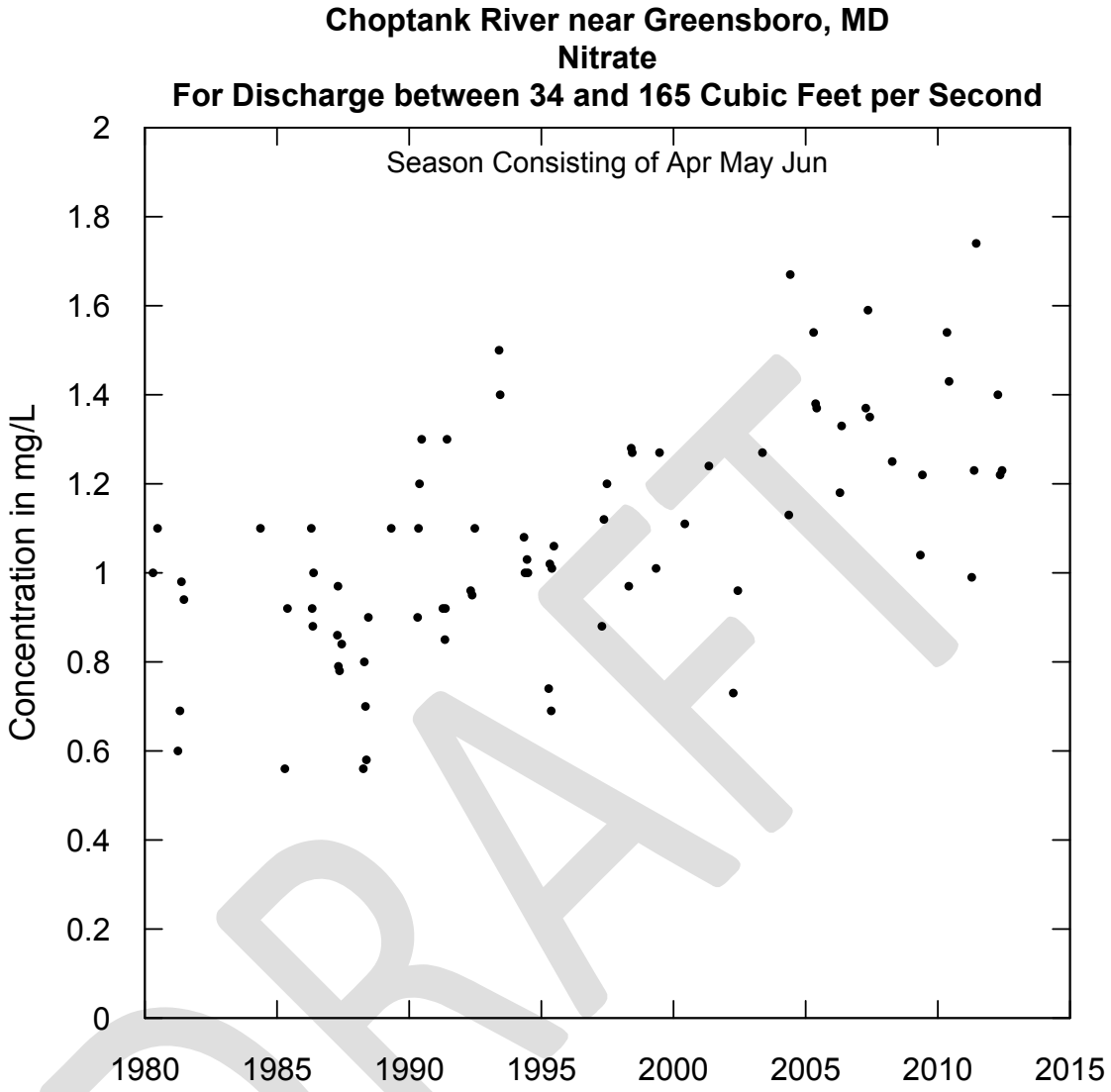


Figure 15. Choptank River near Greensboro, MD, Nitrate, for April, May, June, discharge between 34 and 165 ft^3/s.

Note that the graphic is entirely self-labeled, with the station name, parameter, season, and discharge range all included in the figure title. This can be very useful when generating many plots, assuring that the specific set of conditions used for making the plot are not forgotten later on. It happens that the selected lower and upper bound on discharge used here are the 25th and 75th percentile on the flow duration curve for the full data set. This flow duration information is determined by the

function `flowDuration`, which is described below. The interpretation that can be taken away from this figure is that in this mid-range of discharge, the trend in concentration over the 33 years has been rather consistently upwards. In contrast to this plot a different command can be given to produce a graph (Figure 16) of all the concentrations above 165 ft^3/s. The command is:

```
plotConcTime(qUnit=1,qLower=165, concMax=2)
```

Note the addition of the argument `concMax = 2`. This is done to assure that the maximum value on the y-axis would be 2 mg/L like the scale used in Figure 15. Setting the upper limit on the vertical axis enables the reader to compare levels and/or trend slopes across multiple graphs in a given report.

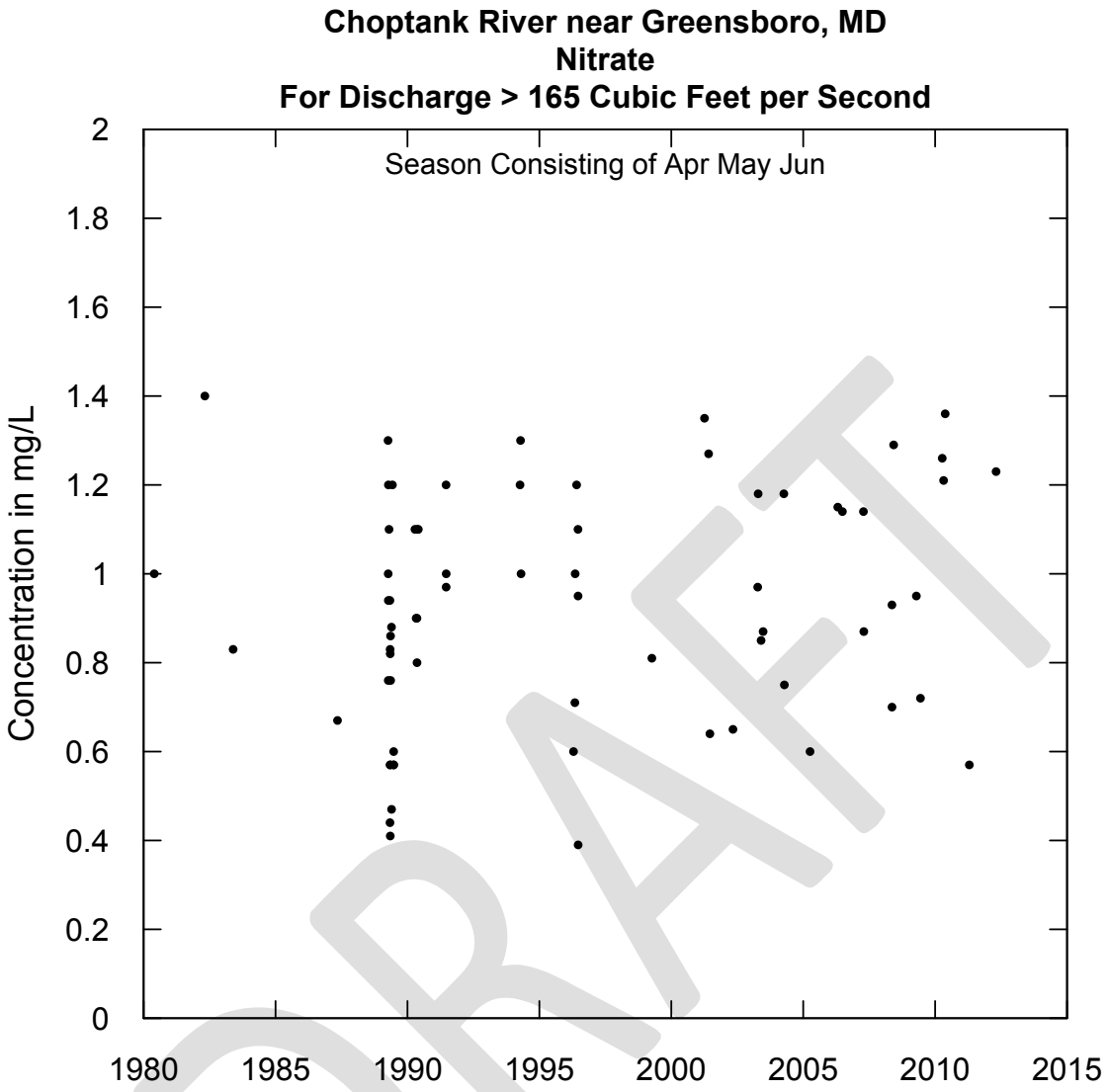


Figure 16. Choptank River near Greensboro, MD, Nitrate concentration for months of April - June, for discharge greater than 165 ft^3/s.

What we see here is that there is really no appearance of a trend in concentration for this season and discharge range, and that concentrations in this discharge range in the later years of this record are lower than the concentrations that occur at lower discharges (as seen in the previous figure). These observations lead to a hypothesis that agricultural practices in this watershed are continually causing

increased loadings of nitrate to the groundwater system. That increase is then expressed via the surface water quality at moderate streamflow, when most of the stream water is derived from the groundwater system. During higher flows, however, the pathways for nitrate are more directly through surface water flow to the stream, and it appears that improved agricultural practices may be effective in limiting the input of nitrate during these events. A later section of this report (Exploring model behavior and adjusting model parameters) contains examples of how these various types of trends (by season or by flow class, or both) can be identified and depicted.

flowDuration

This function is not a graphical function, but is very useful in setting up graphical functions. It provides the user with context about the range of discharge variables that are common and those that are extreme, for the record as a whole or for a particular part of the year. Figure 17 presents the output from the command:

```
flowDuration(qUnit = 1)
```

```
Flow Duration for Choptank River near Greensboro, MD


Flow duration is based on full year


Discharge units are Cubic Feet per Second
    min      5%     10%     25%     50%     75%     90%     95%     max
   0.35   11.00   16.00   33.00   85.00  163.00  290.00  462.00 8700.00
```

Figure 17. Output from flowDuration function.

The `flowDuration` function is designed not only to describe the flow duration curve for the entire year but also has the ability to define it for particular parts of the year. For example, we see here that 33 ft^3/s is the 25th percentile on the full annual flow duration curve. Where does it rank for the

season graphed in Figure 15? Using all of the arguments in flowDuration this can be determined, the command would be:

```
flowDuration(centerDate = "05-16" , qUnit = 1 , span = 45)
```

The argument `centerDate` specifies the month and day that are at the center of the time span of interest (May 16, being the central date of the April, May, June period), `qUnit` specifies that the results are to be reported in ft^3/s, and the `span` argument is half of the width of the period of interest. In this example, the days included in the computation are the centerDate plus those days that are less than or equal to 45 days on either side of it (for a total of 91 days). The output shown in Figure 18 reflects all the choices made through the selection of these arguments when giving the results.

```
Flow Duration for Choptank River near Greensboro, MD


Flow duration period is centered on May 16
And spans the period from April 1  To June 30


Discharge units are Cubic Feet per Second
   min     5%    10%    25%    50%    75%    90%    95%    max
   8.6   30.0   40.0   65.0  112.0  190.0  336.0  526.0 4170.0
```

Figure 18. Output from flowDuration function, with span = 45 days and center date is May 16.

Thus we can see that for this portion of the year, a discharge of 33 ft^3/s is slightly above the 5th percentile of the flow duration curve, rather than the 25th percentile for the full annual distribution.

plotConcQ

A fundamental part of any analysis of surface water quality is to develop an understanding of the relationship between discharge and concentration. This relationship lies at the center of the WRTDS model as well as other commonly-used approaches to water quality analysis such as LOADEST (Cohn

and others, 1992) or the Seasonal Kendall test on flow-adjusted concentrations (Hirsch and others, 1982). A scatterplot of this relationship is produced using the function `plotConcQ`. The graphic shown in Figure 19 was created with the command `plotConcQ()`.

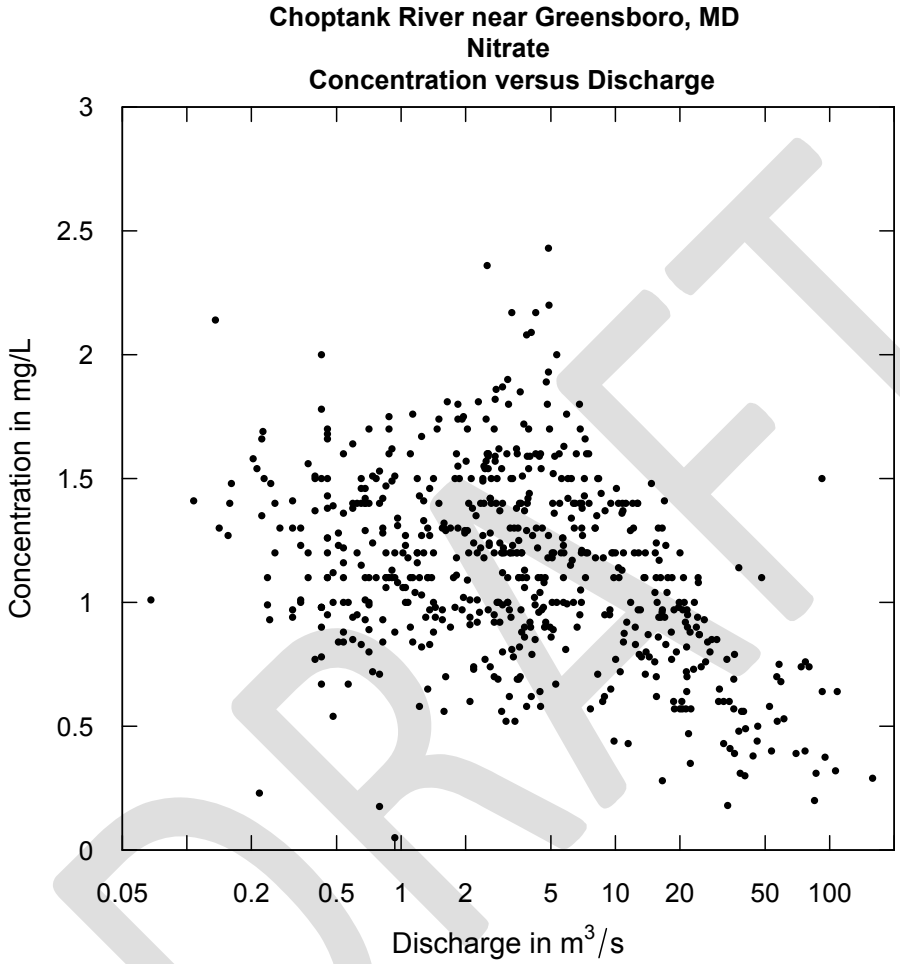


Figure 19. Concentration versus discharge, Choptank River near Greensboro Maryland, Nitrate.

The key arguments that are available to modify this plot (other than those that affect labels, fonts and colors) are these:

- `qUnit`, which determines the units for plotting discharge values.

- `logScale`, if `TRUE` the vertical axis (concentration) is a log scale, if `FALSE` (the default value) it is an arithmetic scale and goes to zero.
- `concMax`, which sets the maximum value for the vertical scale, which can be useful when there is reason to produce a set of similarly scaled plots (say across multiple sites), the default is that the program will set the maximum based on the actual maximum value.
- `concMin`, sets the minimum value for the vertical scale. It is only used when `logScale=TRUE`. The default, when `logScale = TRUE` is that it is automatically set based on the data. When `logScale = FALSE` it is always zero.

Using the `logScale` option can be very helpful because the graph is then presented in the same space in which the WRTDS model will be fitted (log of concentration versus log of discharge) and the common functional forms used in LOADEST or related models will always be linear or quadratic when plotted this way. For example, Figure 20 is produced with the command: `plotConcQ(logScale=TRUE)`

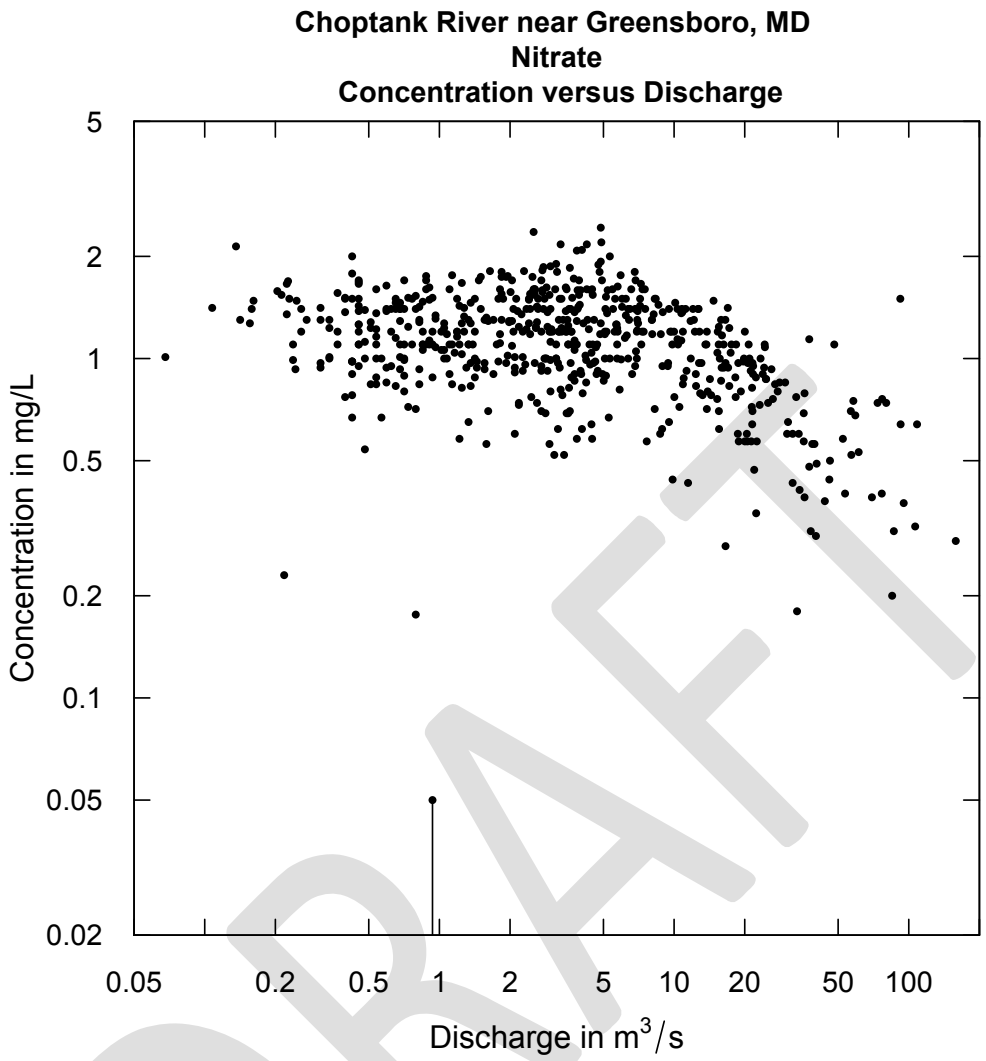


Figure 20. Concentration versus discharge, with concentration on a log scale, for the Choptank River near Greensboro Maryland.

Plotting in this manner can often be helpful in identifying a clear characterization of the relationship between discharge and concentration. For example, in this case it shows rather clearly that there is little systematic relationship between concentration and discharge for low discharge values, up to a level of about 5 m^3/s. Then, beyond that discharge there is a substantial and fairly linear downwards slope. This suggests that base flow water has a rather constant concentration, in the range

of 0.5 to 2 mg/L, but as storm flow begins to enter the system (either surface runoff or shallow ground water movement during and just after precipitation) the new water appears to have a lower nitrate concentration than the base flow water, resulting in a dilution effect. It is likely that neither a parabola nor a linear relationship (in log-log space) would be a good representation of this relationship. Just like `plotConcTime`, this graphic can be used to show data from any specified PA, by using the `setPA` function. This can be very helpful in exploration of seasonal differences in the flow versus concentration relationship.

plotFluxQ

This function produces a graphic that is very closely related to the one shown in Figure 20. It simply presents the data set as flux values rather than as concentrations. For example, this same data set can be plotted with the command: `plotFluxQ(fluxUnit=4)` and the results are shown in Figure 21. The choice of units, in this case thousands of kg/day, is a matter of personal preference.

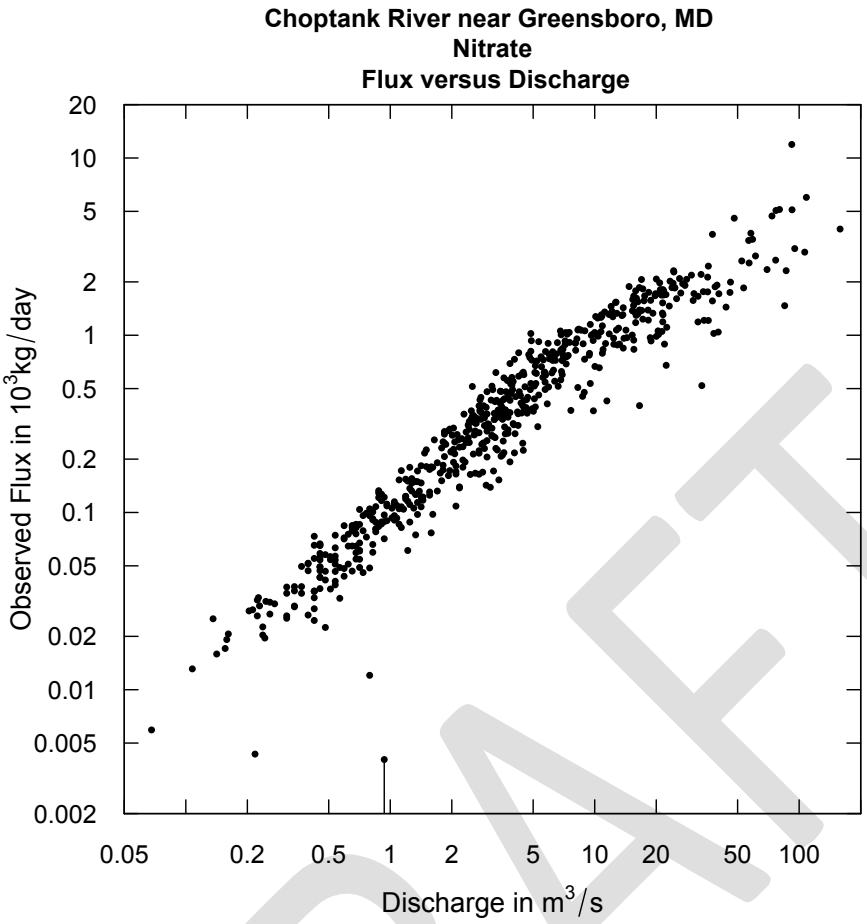


Figure 21. Flux versus discharge plot, Choptank River near Greensboro, MD

This plot shows the same change in slope that is seen in Figure 20. It demonstrates that flux does continue to rise with increasing discharge, but the slope declines above about 5 m^3/s.

boxConcMonth

This graphical function, which produces boxplots by month, is a simple way to characterize the amount of seasonal variability in the data and learn, at a glance, what times of the year have particularly high or low concentrations. Figure 22 is an example of a situation with a very strong and rather complex seasonal pattern (it is based on data from the Iowa River at Wapello Iowa, a watershed with very extensive corn and soybean agriculture). Note that the boxplots used in EGRET all follow the

standard conventions for the length of the box and the length of the whiskers as defined in the R-documentation for the function boxplot (enter `?boxplot.stats` in the console during an R session).

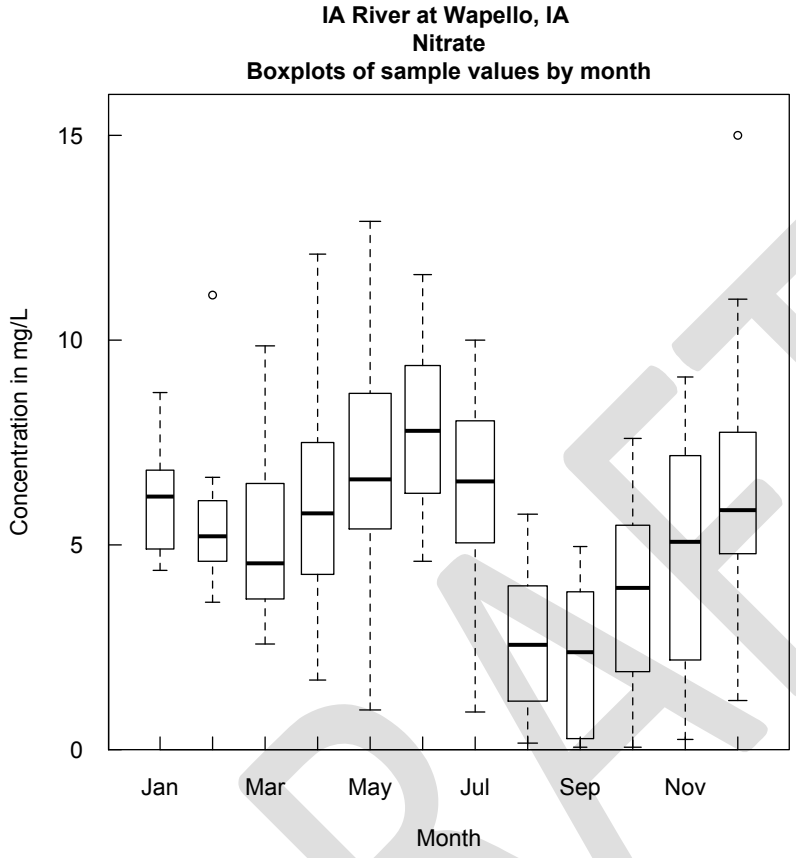


Figure 22. Boxplots by month for the Iowa River at Wapello, IA for nitrate.

It shows a pattern of very high nitrate concentrations during the spring period of high runoff, but moderately high concentrations throughout the colder months of the year (November - March) and relatively low concentrations in the late summer (August and September). This is a result of low discharge and with high temperatures, which causes denitrification to be very effective at removing nitrate from the river.

The boxplots presented here use the plotting convention that the width of the box is proportional to the square root of the number of samples represented by the box. This makes it very clear if there are

large differences in the intensity of samples across the different months of the year. In this case, we can see that September, November, January and February have somewhat fewer samples than the other months. The month with the greatest number is May (37 samples) and the month with the least is September (15 samples). This plot can alert the hydrologist to situations that require considerable care in data analysis because of great differences in sampling intensity, for example sites with virtually no winter sampling.

boxQTwice

This graphical function only shows information about discharge data. It produces two side-by-side boxplots of discharge (on a log scale). The first shows the discharges at which the samples in the data set were taken. The second shows the full population of mean daily discharge values for the entire period of record that will be used in the WRTDS analysis (typically this should be a period that starts with the first water year of sampling and ends with the last water year of sampling). If the sampling strategy for the water quality samples were either random or uniform (e.g. sample once every 14 days) then the two boxplots should be very similar to each other, certainly similar in terms of median values and upper and lower quartiles (the bounding lines on the box). From the standpoint of being able to make accurate assessments of flux (by WRTDS or other methods) it is desirable that the sampling strategy place more emphasis on collecting samples at high discharge. Figure 23 is an example showing a sampling pattern that is well suited to obtaining accurate flux estimates. The lower quartile, median, and upper quartile of the distribution of sampled discharges are all offset higher than the discharges in the full mean daily discharge record. Also, the very highest sampled discharge is actually the third highest mean daily discharge value of the period of record and the mean daily discharge on the highest day is only 36 percent higher than the highest sampled day. This type of plot can be very helpful in identifying those cases where high discharge days are seriously under-sampled, and as a consequence

the fluxes estimated in those cases should be treated with a high degree of caution. These boxplots also use the convention of box width being proportional to the square root of the sample size.

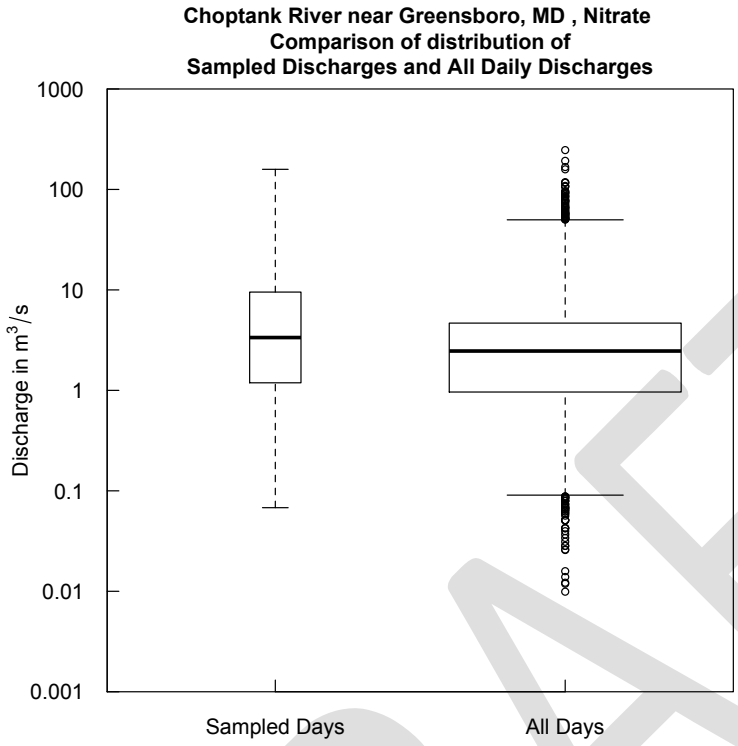


Figure 23. Output from the function boxQTwice for Choptank River near Greensboro, MD.

multiPlotDataOverview

The graphic produced by `multiPlotDataOverview` is single multipanel plot that incorporates the results produced by the four specific plotting functions: `plotConcQ, plotConcTime, boxConcMonth, and boxQTwice`. Figure 24 is an example using nitrate data from the Iowa River at Wapello, IA. At a quick glance one can learn several things about the data set: concentration increases with discharge but only up to a point, and then shows some indication of decreases at the highest discharges (dilution with lower concentration precipitation water), the variability of concentration in log space is much greater for low discharges than for high discharges, there is no easily discernible trend,

the concentrations are highly seasonal with very low values in the late summer and very high ones centered around April, the sampling is fairly well distributed across all months, and well distributed across the range of discharges with some bias towards sampling of higher discharges (which is a desireable situation, as discussed above). All of the component plots can be used with a PA less than the full year, thus, `multiPlotDataOverview` can be produced for any PA and will be labeled accordingly.

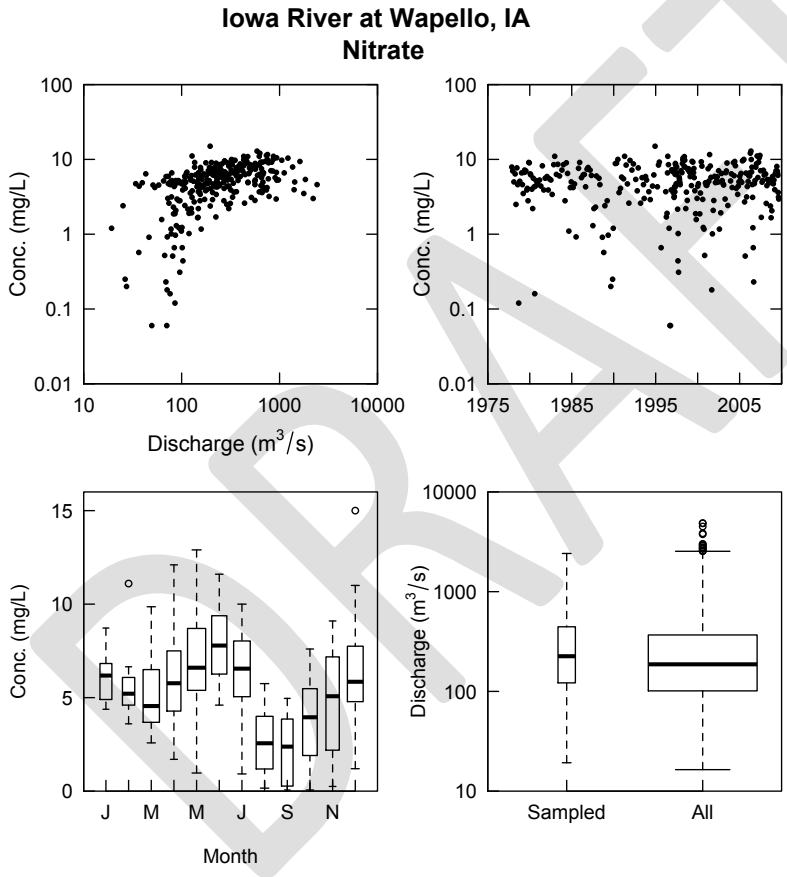


Figure 24. Output from multPlotDataOverview function for nitrate data from the Iowa RIver at Wapello, IA.

WRTDS analysis of water quality data

Overview

WRTDS (Weighted Regressions on Time, Discharge, and Season) is a method for analysis of water quality data sets, which can be used to characterize the status and trends in concentration and flux. For an extensive discussion of the motivations and design of the WRTDS method see Hirsch and others (2010). The method can be used for a variety of purposes. These include: estimating long-term changes (trends) in average concentrations and average fluxes (both annually and for some selected PA), estimating actual mean concentration or fluxes for specific years or specific PA's within the year, estimating mean concentrations or mean fluxes over some specified period such as a decade, and in addition to provide insights into the change in system behavior that may lead to a better understanding of the causative mechanism behind the trends that are observed. The method requires the availability of measured concentrations of the constituent of interest, and a complete record of mean daily discharge for some period of record. The method was designed for data sets with two hundred or more measured concentration values that span a period of a decade or more. However, testing has shown that it in some cases it can produce reliable estimates of mean concentrations or mean fluxes with data sets as small as about 60 samples spanning periods as short as a decade, but doing so requires special settings on some of the arguments of the `modelEstimation` function (described below). The method is not appropriate for small flashy watersheds where discharge at the streamgage commonly changes by an order of magnitude or more within a given day, although it can be appropriate for rivers that are subject to regulation at sub-daily time scales. The discharge data set must cover the entire period of water quality data being used, although it should not be more than a few months longer than the water quality record. Using a discharge record that extends substantially before and/or after the period of the water quality record will result in highly unreliable estimates for the years before and/or after the water quality record.

Smoothing methods, such as WRTDS, should never be used to make extrapolations. A good rule of thumb is to have the discharge record start at the beginning of the first water year for which there are water quality samples and end at the end of the last water year for which there are water quality samples. All of the sample data is stored in the `Sample` data frame, the discharge information is stored in the `Daily` data frame, and the metadata is stored in the `INFO` data frame (see the Data Entry section of this report).

The WRTDS method creates a highly flexible statistical representation of the expected value of concentration for every day in the period of record and then uses that representation to produce four daily time series for the period of record. These are daily concentration, daily flux, flow-normalized daily concentration, and flow-normalized daily flux. The flow-normalized values are intended to describe the changing state of the system over time, by integrating out the influences of variations in concentration or flux that arise from the day-to-day variations in discharge. In contrast, the non-flow-normalized versions of these variables are estimates of what actually happened on each day and, as such, they are highly influenced by the actual discharge that happened that day.

Estimates of concentration and flux

The WRTDS model can be thought of as a smooth surface that describes $E[C] = w(Q,T)$ where C is concentration (in mg/L), $E[C]$ is the expected value of concentration, w is a function which depends on two variables, Q (discharge in m^3/s) and T (time expressed in decimal years). This function can be illustrated in the form of a contour plot, where the horizontal axis is time, and the vertical axis is discharge (shown on a log scale) and the contour plot shading is based on the value of $E[C]$. The graphic shown in Figure 25 represents the estimates of w over a rectangular grid of Q and T values using chloride concentration in the Milwaukee River at Milwaukee, Wisconsin as an example. The figure indicates that over this 35 year period concentrations have been highest at low flows, that there is

seasonality such that, for a given discharge concentrations are higher in the winter than in the summer, and that there is an overall upwards trend in concentrations across most of the range of discharges and seasons. This particular graphic is produced by the `plotContours` function, which will be described in detail in the section "plotContours".

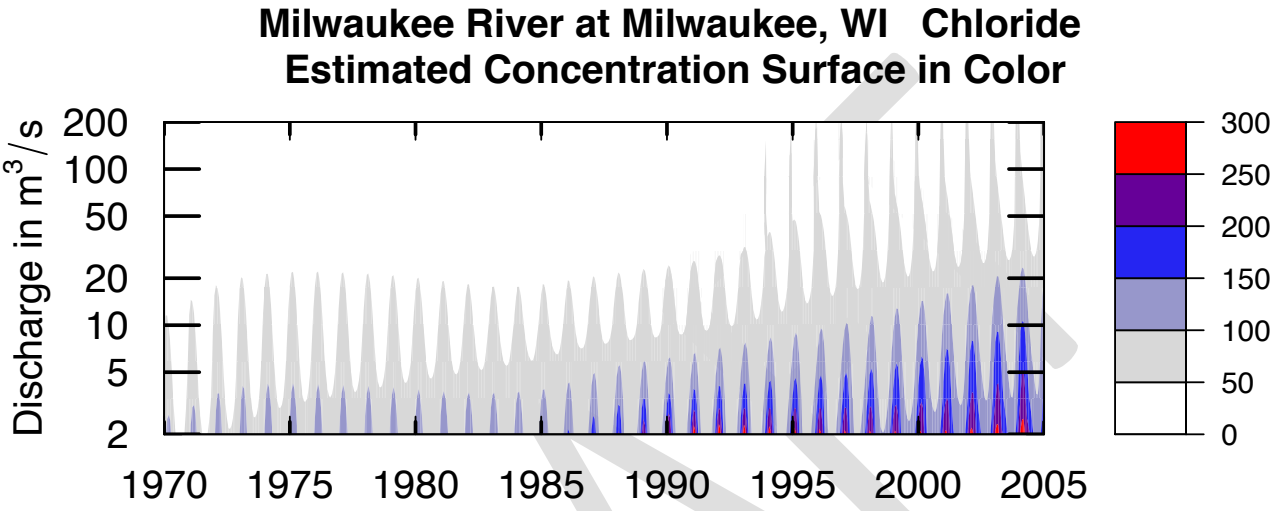


Figure 25. Contour plot of expected value of chloride concentration as a function of time and discharge, Milwaukee River at Milwaukee, WI

In the EGRET code, the discharge values for the grid are 14 values that are equidistant in log space. They run from a discharge value about 5 percent below the minimum discharge in the daily record to a value about 5 percent above the maximum discharge in the daily record. This is defined more precisely below in the discussion of the `surfaceIndex` function. The grid values for time are spaced 0.0625 years apart ($1/16^{th}$ of a year). The full data set used in this example actually extends beyond the bounds of the graphic shown, consisting of 673 time steps by 14 discharge steps for a total of 9422 nodes, of which 4616 fall within the space covered by this graphic. At each node of the grid the estimates of E[*C*] are made as follows. A weighted regression model is estimated. It takes the form:

$$\ln(c) = \beta_0 + \beta_1 q + \beta_2 T + \beta_3 \sin(2\pi T) + \beta_4 \cos(2\pi T) + \varepsilon \quad (6)$$

c is concentration in mg/L, q is ln(Q) where Q is mean daily discharge in m^3/s, T is time expressed in decimal years, and ε is the error (unexplained variation). Because equation 6 is fitted at each node there are unique estimates of each of the β values and also a unique value of the standard error at each node. The EGRET program does not save the individual β values but does save the estimate of ln(c) at that node and the standard error at that node. It is important to recognize that although the form of the equation is written as if ln(c) is linear in q and T varies seasonally as a perfect sine wave. However, because the coefficients vary throughout the Q,T space, the linearity or sine wave form is only true locally. The estimation method assures that the estimates of ln(c) vary smoothly with q and T but are not constrained to linear or sine wave characteristics.

This equation is actually fit in the form of a weighted Tobit model (Tobin, 1958), where the c values can be individual values of concentration, or they can be intervals such as (0,0.05) where 0.05 is the minimum reporting level, (one would typically call such a value of concentration “less than 0.05"), or they could be some other interval such as (0.04,0.05) which might arise when the analyte in question is the sum of two individual analytes (see Appendix A Section 3.4 for a discussion of data entry for these censored cases).

The weights on each of the individual observations in the data set are determined on the basis of three metrics of distance between the node and the specific observation. The distance metrics are distance in time, distance in q, and distance in season (which is measured in units of years, but only considers the fractional part of the time separation in years). For example, if we compare a sample value with q and T values of 3.0 and 1995.0 respectively, to a grid point with q value of 3.8 and a T value of 1997.25, then the distance in log discharge would be 0.8, the distance in time would be 2.25 years and the distance in season would be 0.25 years. Weights are associated with each of these three

distances measures, using the Tukey tri-cubed weight function (described above where the function `makeAnnualSeries` is described in the Flow History Analysis section). The half window widths (the *h* value in the formula for the weights) have default values of 2 (in log discharge units), 10 years, and 0.5 years. The overall weight for any observation is the product of the three weights, so a weight of zero for any of the three metrics results in an overall weight of zero. For any given node on the grid, the estimate of ln(*c*) is computed (using the R function `survReg`, which is an implementation of "survival" or Tobit regression). In the EGRET code this estimated value is known as `yHat`. In addition, the scale parameter of the survival regression is also stored for every node. The scale parameter is equivalent to a standard error (SE) of the residuals in an ordinary multiple regression. This error measure is known as `SE` in the EGRET code. To determine the expected value of *c*, the `yHat` value must be multiplied by a bias correction factor (BCF) to account for the fact that the model is estimating ln(*c*) rather than estimating concentration itself and the errors in these estimates of ln(*c*) are assumed to be normally distributed. The BCF at each grid point is $\exp(SE^2/2)$. The third result that is stored is E[*c*], which is called `concHat` in the EGRET code. These three results are related by this formula:

$$\texttt{concHat} = \text{BCF} * \exp(\texttt{yHat}) \tag{7}$$

Figure 26 show each of these three surfaces (concHat, yHat, and SE each as a function of DecYear and Q). The bottom panel Figure 26 is shows a three-year segment of the full history shown in Figure 25. The following are several observations about these surfaces.

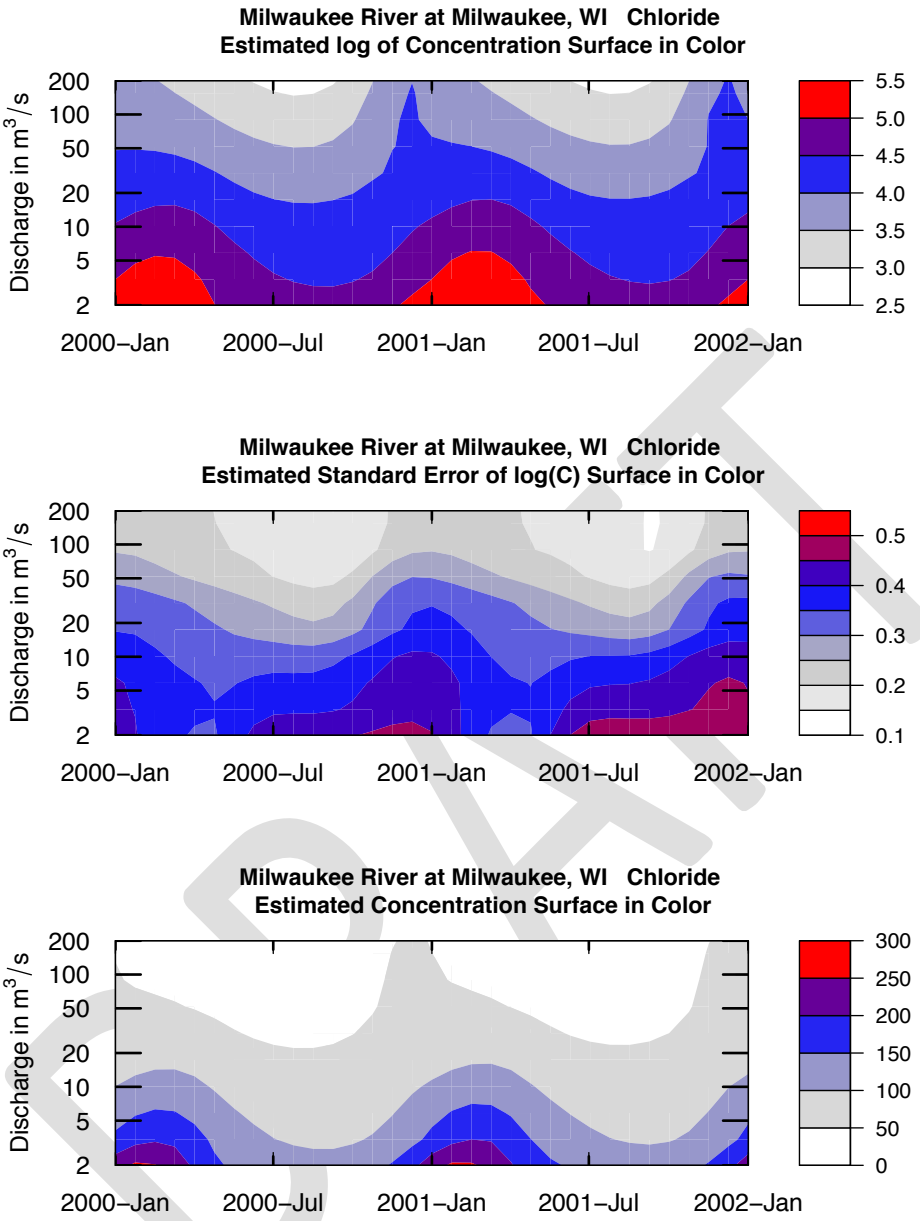
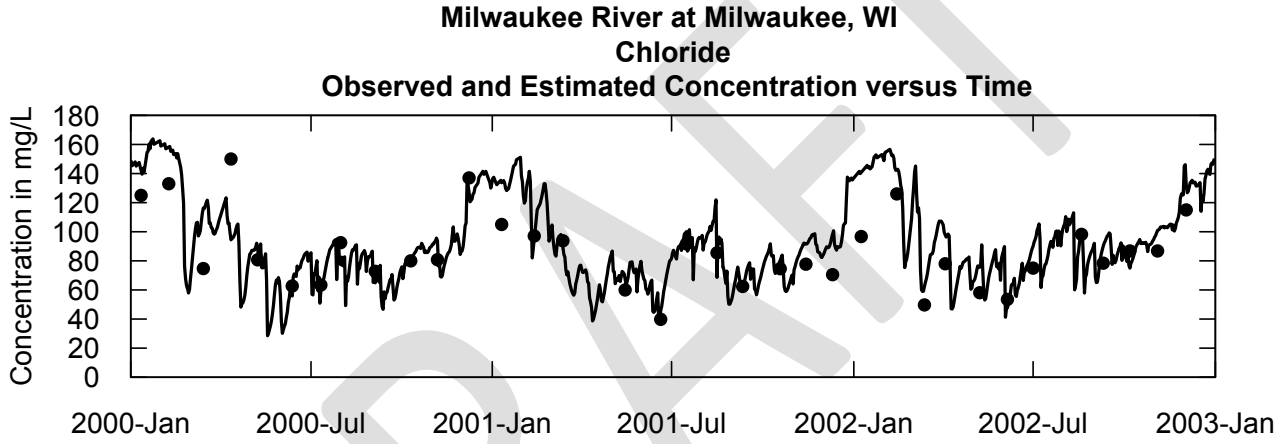


Figure 26. Contour plots of fitted WRTDS model for Milwaukee River Chloride data, showing the years 2000-2003. Upper panel is the estimate of the ln(*c*) surface, middle panel is the estimate of the standard error and bottom panel is the estimate of concentration.

- All of the surfaces are relatively smooth; this is a consequence of the weighted regression smoothing approach. Modifying the half-window widths would change the degree of smoothing in these surfaces. The section "Exploring model behavior and adjusting model parameters" considers the basis for selecting appropriate half-window widths.
- They all show a seasonal pattern, but that pattern evolves slightly over time. In general, that pattern is one of higher concentrations in the winter and lowest in the summer. The highest concentrations are focused during times of very low discharge in the months of January, February and March. In all seasons, concentration tends to decrease as discharge increases.
- The variability (shown in the middle panel as the plot of estimated standard error of log(*C*)) shows clear differences across a range of discharges and seasons, indicating that an assumption of homoscedastic residuals is not appropriate. This point is an important distinction between WRTDS and LOADEST (Cohn and others, 1992; Runkel and others, 2004). In LOADEST, the errors are assumed to be essentially constant across all seasons and discharges, and as a consequence, the BCF they use is virtually constant across all seasons and discharges. The WRTDS model recognizes and uses these very substantial differences in the SE to compute the estimated concentrations.

The WRTDS model uses the characterization of the E[*c*] surface to make estimates of concentration for every day in the period of record. These individual daily estimates of concentration are made through a bi-linear interpolation of the `concHat` value from the grid of estimates, using the values of *q* and *T* specific to that day. If the model assumptions of WRTDS were perfect, then these estimates would each be an unbiased estimate of concentration for that specific day. However, these estimates, taken in aggregate, will not exhibit as much variability as a real record would. As with all regression-based estimates, they have the property that they “regress to the mean.”

Each of these daily estimates of concentration is also used to compute a daily estimate of flux. Flux for each day, in units of kg/day, is computed as `concHat` * `Q` * 86.4 where `concHat` is the daily estimate of concentration (in mg/L), `Q` is the mean daily discharge (in m^3/s), and 86.4 is the unit conversion. Figure 27 shows a 3-year example of the concentration and flux outputs of the model and compares the model results to the actual measurement. In EGRET these daily estimates of concentration and flux are both stored in the `Daily` data frame and are named `Daily$ConcDay` and `Daily$FluxDay` respectively.



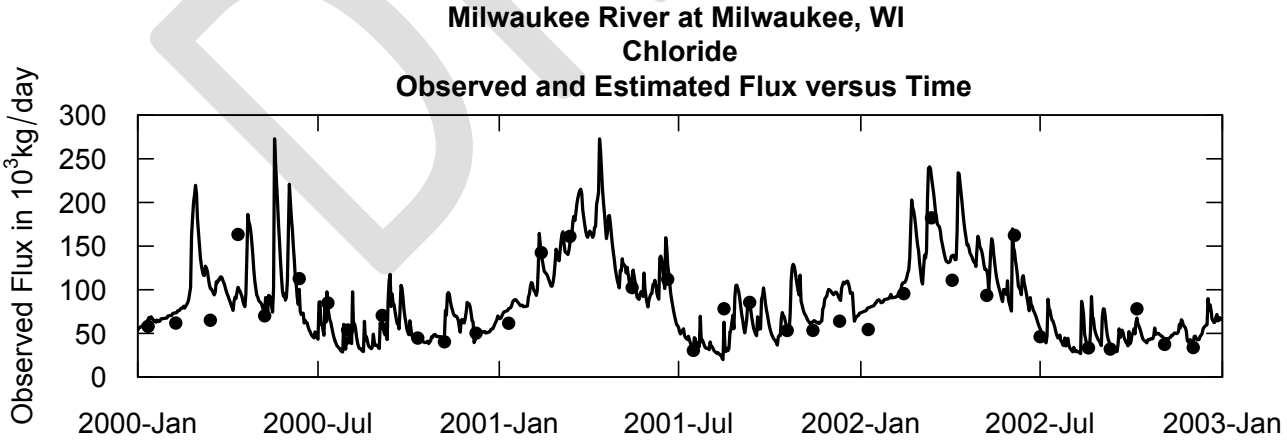


Figure 27. Observed and estimated concentrations (upper panel), observed and estimated fluxes (lower panel). Chloride, Milwaukee River. In each panel, the dots represent the observations and the line represents to WRTDS estimates for all of the days.

Estimation of flow-normalized concentration and flux

Estimates of daily concentration and daily flux are of great value and importance in terms of knowing the actual history of water quality in a river. Particularly where there is an interest in understanding the water quality or ecological condition in a receiving water body such as an estuary, lake, or reservoir the variable of interest would be the history of flux integrated over time periods such as months, seasons, or years. Also, when the interest is in the concentrations of a pollutant that may have impacts on receptors such as biota or water supply intakes then the history of concentration will be of interest. However the history produced by the model will not describe the frequency of exeedances of water quality criteria or standards because the concentration estimates will have less variability than real records would. The concentration or flux estimates (Daily$Conc and Daily$Flux) can be very strongly influenced by the particular time history of flow conditions. For example, for a pollutant for which concentration increases with discharge, a high flow period of a year or two near the end of the period of record can suggest deteriorating water quality. For those interested in evaluating the effectiveness of pollution control efforts, these types of results can seriously confound the analysis. The variability in concentration or flux that is related to discharge can overwhelm a true signal of change. Discharge-driven variability creates a large amount of apparent "noise," thus making the identification of trend virtually impossible. For those seeking information about "progress" or "effectiveness" or an understanding of how the watershed system is changing, what is needed are time histories that filter out the impact of year-to-year variation in discharge.

The method used to accomplish this in WRTDS is called "flow normalization". It can be described in the following manner.

$$E\left[C_{fn}(T)\right] = \int_0^\infty w(Q,T) \bullet f_{Ts}(Q)\, dQ \tag{8}$$

$E\left[C_{fn}(T)\right]$ is the flow-normalized concentration for time T (a specific day of a specific year)

$w(Q,T)$ is the WRTDS estimate of concentration as a function of Q (discharge) and T (time in years)

$f_{Ts}(Q)$ is the probability density function (pdf) of discharge, specific to a particular time of year, designated at T_s. T_s is restricted to values between 0 and 1, and it is defined as the fractional part of the time variable T (thus T_s is the decimal portion of `decYear`).

Thus, the flow-normalized concentration on a specific day (a specific value of T) is the integral of the fitted estimates of concentration as a function of discharge and time multiplied by the pdf of discharge for that day of the year.

The challenge to operationalizing this function is the specification of the pdf of discharge for each day of the year. In WRTDS, this starts with the assumption that for any given day of the year the distribution of discharge is stationary. This means that, for example, the pdf of discharge for September 9, 2013 is the same as the pdf of discharge for September 9, 1993. If there is a strong reason to believe that discharges have not been substantially stationary over the period of record, then the flow normalization method is not appropriate. From a practical standpoint this suggests that the flow normalization should not be used if major changes in the watershed took place during the period of record that have the potential for causing a substantial shift in the probability distribution of daily discharges for part or all of the year. Examples of such changes could include a large dam or diversion put into operation or taken out of operation, a large new import of water, a large change in consumptive

use of water or large changes in baseflow due to changes in groundwater levels. The presence of dams upstream is not a reason to avoid using this method unless there was a substantial shift in the operations of the dam that changed the pattern of daily discharges (not sub-daily discharges) at the streamgage of interest. Also, dams built or removed farm upstream of the streamgage, controlling a small fraction of the watershed's flow is not a reason to avoid using flow normalization. At present, the changes in discharge due to climate change are not likely to be of sufficient magnitude to invalidate the flow-normalization method but this may become a more important consideration in future years.

A good test of the appropriateness of the method could come from the hydrologist performing the following thought experiment. On September 9, 2013 (for example) what do you think the pdf of discharge is for September 9, 2014? If you say that the history of discharge on all of the past September 9ths would provide a good estimate, then you should be willing to use this procedure. But, if you believe that the pdf for September 9, 2014 differs from the past history in some specific and quantifiable way, then the flow-normalization method should not be used. There are ways to modify the WRTDS method to accommodate this non-stationary case, but the necessary methods have not been incorporated into the EGRET code. Making such enhancements is an important goal for the future of the method.

The other issue that must be resolved to use this method is how to characterize the pdf of discharge for each specific day of the year. There are certainly ways that a continuous, seasonally varying model of streamflow distributions can be characterized, but they require a large number of assumptions and estimated parameters. Given the richness of the discharge data sets that are used in WRTDS (a 20 year record has over 7300 values), it is reasonable to simply use the full historical sample as a representation of the pdf. In the case of a 20-year record, this means that we would assume that the pdf for September 9 is the 20 observed values, each assigned a probability of 0.05. The resulting pdf by itself is not very realistic (having zero probability for all values other than these), but when taken

together with a similarly constructed pdf for September 10, September 11, etc. the collection of these begins to take on the characteristics of a nearly continuous and smooth pdf. The flow-normalized estimates for successive days can differ from each other by large amounts but WRTDS flow-normalized estimates are aggregated to averages for a specific months, seasons, or years. The approach described here produces time series of annual flow-normalized values that are quite smooth because they integrate over such a large number of individual daily estimates.

In practical terms, how is this computation carried out? If our interest is in the flow-normalized concentration for September 9, 2013, then we use the $w(Q,T)$ function evaluated at T of 2013.690 (because September 9 is 0.690 years from the start of the year), so this becomes a function simply of Q. Then, we assemble the Q values for all 20 of the September 9ths in the record and evaluate $w(Q,2013.690)$ using bilinear interpolation in terms of T and $\ln(Q)$. The average of these 20 concentration values becomes the flow-normalized concentration value for September 9, 2013. It is the expected value of concentration on September 9, 2013, integrating over the estimated frequency distribution of discharge for September 9. This process is repeated for every day in the period of record and the results of the process become the time series of flow-normalized concentrations for the period of record. These daily values can be aggregated to monthly values (by computing a mean of the flow-normalized values for the month) and also aggregated to yearly values (by computing a mean of the flow-normalized values for the year). These monthly values will show strong seasonality and will change gradually over time, but they will be free of any variation due to the occurrence of high or low flow conditions in any given month. Similarly, the annual values will show gradual change over time, but will be free of any variation due to the occurrence of high or low flow conditions in any given year.

The flow-normalized flux is computed in a similar manner, but in this case the random variable of interest is flux rather than concentration. As such, the integral is this.

$$E\left[F_{fn}(T)\right] = \int_0^\infty Q \bullet 86.4 \bullet w(Q,T) \bullet f_{Ts}(Q)\, dQ \qquad (9)$$

The EGRET code computes the flow-normalized concentration and flow-normalized flux for every day of the record and stores these in `Daily$FNConc` and `Daily$FNFlux` respectively.

Fitting the WRTDS model

The fitting of the WRTDS model using the EGRET code can be accomplished through a single function called `modelEstimation`. This function, which uses some unconventional programming techniques, is designed to take information from the `Sample`, `Daily`, and `INFO` data frames and augment versions of each of these as well as create the object called `surfaces`. Even though the user can accomplish this through a single command, this section of the report will briefly describe each of the functions that are called by it, the new data frames returned, and the augmentation of the existing data frames that is accomplished. In describing the process, the discussion will assume that the data frames being used take their standard names: `Sample`, `Daily`, and `INFO` and alternative names are not being used. See "Working with multiple versions of data frames" for more information on the use of alternative names.

The command for conducting the model estimation process is this:

```
modelEstimation(windowY = 10, windowQ = 2, windowS = 0.5, minNumObs = 100,
minNumUncen =50).
```

To invoke the function leaving all five arguments set to their nominal values the command would simply be: `modelEstimation()`. Table 7 explains the 5 arguments that are used in fitting the model.

Table 7. Information about the 5 arguments used in modelEstimation.

Argument	Definition and discussion	Default

		value
windowY	The half window width for the time weighting, measured in years. Values much shorter than 10 usually result in a good deal of oscillations in the system that are likely not very realistic. Values great than 10 may "oversmooth" the underlying trends.	10
windowQ	The half window width for the weighting in terms of ln(Q). For very large rivers (average discharge values in the range of many thousands of m^3/s) a smaller value than 2 may be appropriate, but probably not less than 1.	2
windowS	The half window width for the seasonal weighting, measured in years. When windowS = 0.5 all data points get a non-zero weight, but those close to a half a year away get weights that are virtually zero. For large data sets a value smaller than 0.5 may be appropriate, but should not be lower than 0.25. Values greater than 0.5 cause the importance of the seasonal weighting to be diminished. Setting windowS to a large number such as 10 has the effect of eliminating seasonal weighting.	0.5
minNumObs	This is the minimum number of observations with non-zero weight that the individual weighted regressions will require before they will be used. If there too few observations the program will iterate, making the windows wider until the number increases above this minimum. The only reason to lower this is in cases where the data set is rather small. It should always be set to a number at least slightly smaller than the sample size. Any value lower than about 50 is probably in the "dangerous" range, in terms of the reliability of the regression.	100
minNumUncen	This is the minimum number of uncensored observations with non-zero weight that the individual weighted regressions will require before they will be used. If there are too few uncensored observations the program will iterate, making the windows wider until the number increases above this minimum. The only reason to lower this is in cases where the number of uncensored values is rather small. The method has never been tested in situations where there are very few uncensored values.	50

The modelEstimation function carries out a series of 5 operations in the following order:

- estCrossVal. This function applies the weighted regressions for all the observations in the data set for purposes of model evaluation. It uses "leave-one-out cross validation" to compute, for each of the observations in the Sample data frame, 1) an estimate of the log of concentration, 2) the standard error of the regression, and 3) the unbiased estimate of concentration. For each observation in the data set it runs the weighted regression estimate for that specific discharge and time but with that specific observation left out of the data set. This provides a more realistic evaluation of the model's ability to make predictions. This "leave-one-out cross validation" is appropriate for a method such as WRTDS because the highly flexible nature of the method can be over-fit to the data, particularly to the more extreme values in the data set. For a discussion of this approach to cross-validation see, for example, the discussion of the PRESS statistic in

Montgomery and others, (2012, pp. 151–2). These estimates are added to the Sample data frame and are named: `Sample$yHat` (the estimate of ln(*c*)), `Sample$SE` (the estimate of the standard error of the regression), and `Sample$ConcHat` (the estimate of concentration). These results are used in a number of functions that are introduced later in the section "Exploring the quality of the fitted model."

- `surfaceIndex`. The purpose of this function is to set up the grid over which the WRTDS model will be estimated. The six parameters that define the grid are determined as a function of the information in the `Daily` data frame: specifically the maximum and minimum daily mean discharge values (`Daily$Q`) and starting and ending date of the daily values record (the first and last values of `Daily$DecYear`). These four variables are used to establish the grid used to define the three surfaces that will be stored in the object called `surfaces` (described below). The grid for discharge is equally divided in ln(*Q*) and runs from the minimum value of ln(*Q*) minus 0.05 to the maximum value of ln(*Q*) plus 0.05. This results in a range from 4.877 percent below to 5.127 percent above the range of observed discharges in the full discharge record. The grid for time runs from the start of the calendar year that includes the minimum value of `Daily$DecYear` to the end of the calendar year that includes the maximum value of `Daily$DecYear`. For example, if the discharge record stored in the `Daily` data frame ran from 1982-10-01 to 2012-09-30, then the grid would run from 1982.0 to 2013.0. The grid spacing is 0.0625 years ($1/16^{th}$ of a year) so in this case the time values for the grid would total 497 values (16 per year times 13 years plus one additional grid for the end of the last year). In this case, the total number of nodes to the grid for computing the surface would be 6958 (497 columns times 14 rows). The parameters that define the grid are then stored in the `INFO` data frame. They are called: `bottomLogQ`, `stepLogQ`, `nVectorLogQ`, `bottomYear`, `stepYear`, and `nVectorYear`

(signifying the lowest value, the step between values and the number of values, first for the discharge dimension and second for the time dimension). Also stored in `INFO` at the same time are the 5 specified parameters: `windowY, windowQ, windowS, minNumObs,` and `minNumUncen`. By storing all of these parameters in `INFO` they serve to document how the set of estimates was made.

- `estSurfaces` is the function that fits the model at every one of the grid points defined in `surfaceIndex`. At every grid point it stores three values into a matrix called `surfaces`. The dimensions of `surfaces` are [`nVectorLogQ, nVectorYear`, 3], thus in the previous example the dimensions would be [14, 497, 3]. The first two indices simply go from the smallest to the largest grid values of log(*Q*) and time respectively. The third dimension stores results in this order. The first is the estimated log concentration (`yHat`). The second is the estimated standard error (`SE`). The third is the estimated concentration (`ConcHat`). These three values, at any grid node are related to each other in the following way: `ConcHat` = BCF * exp(`yHat`) where BCF = exp($SE^2/2$). The term BCF is the "bias correction factor". The matrix `surfaces` is used later to create the estimated daily values of concentration, flux, and the flow-normalized versions of these, and to produce the contour surfaces such as those seen in Figure 25 and Figure 26. The `estSurfaces` function calls the function `runSurvReg,` which sets up the survival regression where the estimation is accomplished. The fitting computations are done through the R function `survreg,` which is in the `survival` package using `interval2` censoring (which allows for left censoring and interval censoring) with a `lognormal` distribution assumed for the y variable (which is concentration).
- `estDailyFromSurfaces` is the function that uses the `surfaces` object in conjunction with the individual daily discharge values stored in the `Daily` data frame. For the given values of

DecYear and LogQ, it interpolates values of ConcHat. The value of ConcHat for a given day becomes Daily$ConcDay (in mg/L). This is then multiplied by the discharge and the unit conversion (86.4) to become Daily$FluxDay (in kg/d). The estDailyFromSurfaces function also uses the same interpolation method to compute daily values of yHat (the expected value of ln(c)) and SE (the regression standard error). These are stored as Daily$yHat and Daily$SE. This function also computes the flow-normalized values of concentration and flux for the day and stores them as Daily$FNConc and Daily$FNFlux. The process for computing the flow-normalized series is described above in the section "Estimation of flow-normalized concentration and flux."

- setupYears is the function that takes the contents of Daily and computes water year mean values for Conc, Flux, FNConc, and FNFlux. These annual average values are then placed in a new data frame called AnnualResults. The full set of variables in AnnualResults is shown below in Table 8.

Table 8. Column names for the data frame AnnualResults.

Name of column	What it contains
DecYear	Mean value of Daily$DecYear for all the days included in the year.
Q	Mean value of Daily$Q for all the days in the year (m^3/s)
Conc	Mean value of Daily$Conc for all the days in the year (mg/L)
Flux	Mean value of Daily$Flux for all the days in the year (kg/d)
FNConc	Mean value of Daily$FNConc for all the days in the year (mg/L)
FNFlux	Mean value of Daily$FNFlux for all the days in the year (kg/d)
PeriodLong	The value of paLong used to set up the period of analysis (the length of the PA, in months)
PeriodStart	The value of paStart used to set up the period of analysis (the first month of the PA)

Note that this final step is based on the assumption that the user is interested in results that are organized on the basis of water years. If the results of interest are for some other PA (e.g. a calendar year, a season, a pair of months, a single month) then after `modelEstimation` has been run, the user can call on `setupYears` to summarize the results using some different PA. If, for example, if the user wanted to consider averages for the months April, May, and June, of each year, the command would be:

```
AnnualResults <- setupYears(paLong = 3, paStart = 4)
```

Or if the interest is in just the month of May it would be

```
AnnualResults <- setupYears(paLong = 1, paStart = 5)
```

There is no need to re-estimate the model (a somewhat time consuming step) if the user simply wants to change the PA that they use to summarize the results. The user generally does not need to run the `setupYears` function because the individual functions that present the results as graphs or tables (defined the subsequent section “Displaying and managing WRTDS model results”) each make this computation using whatever PA the user selects.

Given the amount of computer time and effort involved in reaching this point in the analysis, it is wise to save the workspace at this stage. The instructions for doing this are given above in the section "Saving the workspace for future use". The command is simply

```
saveResults(savePath)
```

Displaying and managing WRTDS model results

Computing monthly results

If monthly results are desired rather than annual or seasonal they can be generated using the command: `MonthlyResults<-calculateMonthlyResults()`. The data frame `MonthlyResults` is similar in structure to `AnnualResults`. It contains mean values for each month for discharge, concentration, flux, flow-normalized concentration, and flow-normalized flux. It also has columns for

month (values of 1 through 12 with 1 being January), year (the calendar year) and DecYear (the decimal year value for the midpoint of the month). There are no functions particularly designed to display the content of `MonthlyResults`, but they can certainly be plotted or printed using standard R functions for plotting or printing the content of a data frame. The units for the results in `MonthlyResults` are m^3/s for discharge, mg/L for concentration, and kg/day for flux.

Issues of large data gaps - using the `blankTime` function

When the concentration record has a large data gap, the WRTDS estimates during the time of the data gap are likely to be highly unreliable. Because WRTDS makes no prior assumptions about the shape of the time trend, the computations can create large oscillations during long data gaps. These are just numerical artifacts. A data gap of two years or less (regardless of the overall record length) is generally no problem, but as they become longer it may be prudent to use the `blankTime` function to eliminate the results for the gap period. The `blankTime` function should also be used if there is a period of a few years during which the sampling frequency is very low (say fewer than six observations per year). If there is a long data gap or period of very sparse data, the `modelEstimation` step should be run as usual, but after it has been run the `blankTime` function should be run. What this function does is replace all of the estimated values (`yHat, SE, ConcDay, FluxDay, FNConc, FNFlux`) in the `Daily` data frame during the blank period with `NA` (missing value indicator). The user must specify the starting and ending date of the gap. It may be prudent to make that blank period a few months longer than the actual gap and it may also be prudent to start and end it with the starting and ending dates of water years, if water years are going to be the basis for annual summary computations. Regardless of how the blank period is set by the user, any water quality data that may exist during that period will be used in the estimation process to inform the model, but the model is simply not used to produce daily estimates during this blank period because they are likely to be highly unreliable. The discharge data during this

period are still used along with the rest of the discharge data for purposes of making flow-normalized estimates. It is also possible to use `blankTime` more than once on a given data set if there are multiple data gaps. The command is:

```
Daily <- blankTime(startBlank, endBlank)
```

The arguments `startBlank` and `endBlank` must both take on the form of a date expressed in yyyy-mm-dd form and must be inside of quotation marks. For example, if the hydrologist's judgment is that results for water year 1980 through water year 1989 should be blanked out, then the blank period might be defined as 1979-10-01 to 1989-09-30. In this example the commands would be:

```
startBlank<-"1979-10-01"
endBlank<-"1989-09-30"
Daily<-blankTime(startBlank,endBlank)
```

Or alternatively, it could be done as a single command.

```
Daily<-blankTime("1979-10-01","1989-09-30")
```

The result of the command is that a new version of `Daily` (with `NA` values inserted) is simply substituted for the old version. Any subsequent commands to display annual results as graphs or tables will be based on this new version of Daily and the periods with NA values will be reported as missing in the graphical or tabular output.

Plotting annual results

The function `plotConcHist` is used to plot the annual average concentration and annual flow-normalized concentration. The annual average concentration will be displayed as individual points (plotted at the mid-point of the PA). The flow-normalized results will be presented as a smooth curve (in green) even though they are computed for a single point in time for each year. This graphical

convention simply emphasizes the relatively smooth nature of the flow normalized concentration record in contrast with the annual average concentration record.

This function can be used to plot these values for any PA and the title will always indicate the PA that was used. The user determines the PA by using the function `setPA` prior to running `plotConcHist`. If the `setPA` command has not been used previously for the given data set then the function will produce values for the water year. To select a different PA the command would be:

```
INFO <- setPA(paStart, paLong)
```

So, for example to consider the months of April, May and June, the command would be:

```
INFO <- setPA(paStart=4, paLong=3)
```

This information about the PA will be carried within the `INFO` data frame and will thus be used by the other functions described in this section (`plotFluxHist`, `tableResults`, and `tableChange`) but can be changed by the user at any point in their session. These instructions about the setting up the PA apply in exactly the same manner to all of these functions.

After setting the PA the command for making the plot, in its simplest form, is just `plotConcHist()`. With the arguments that would typically be used to further refine the graphic, the command is:

```
plotConcHist(yearStart, yearEnd, concMax, printTitle, plotFlowNorm)
```

Table 9 describes these arguments:

Table 9. Commonly used arguments for `plotConcHist`.

argument	meaning	default
`yearStart`	The starting year for the graph, typically expressed as integer values (e.g. 1980). Note that left margin of the graph will probably be an earlier year, but the data will commence with the first yearly value after `yearStart`.	NA, which causes it to start at or a few months before the first year of record
`yearEnd`	The ending year for the graph. This should typically be the start of the calendar year after the last annual value to be plotted. The right edge of the graph will typically be after `yearEnd`	NA, which causes it to end at or just after the last year of record
`concMax`	If specified, this defines the upper bound on the vertical axis	NA, which causes the

	of the graph. This can be very useful if there are going to be multiple graphs (for different sites) of the same constituent. The use of the same vertical scale facilitates comparisons across sites.	graph to be self-scaling.
printTitle	If TRUE the title is printed above the graph. If the illustration is for a publication, where this information would go into the caption, then FALSE would be the best choice.	TRUE, title is printed
plotFlowNorm	If TRUE the graph shows the annual concentrations as circles and the flow-normalized values as a green curve. If FALSE, it only shows the annual concentrations.	TRUE, both are shown

The function `plotFluxHist` is used to plot the annual average flux and annual flow-normalized flux. The command, in its simplest form is just `plotFluxHist()`. With the arguments that would typically be used to further refine the graphic, the command is:

```
plotFluxHist(yearStart, yearEnd, fluxUnit, fluxMax, printTitle, plotFlowNorm)
```

These arguments are identical to the arguments listed above for `plotConcHist` except that `fluxUnit` is added and in place of `concMax` there is the argument `fluxMax`. The argument `fluxUnit` defines the units to use for the vertical axis. To review these the user can give the command `fluxUnitCheatSheet()` and all of the options will be listed. The list is also provided in Appendix B section 3.4. The default is `fluxUnit=9` which is millions of kg/year. If those are the desired units then the argument `fluxUnit` can be left out. If, for example the user wanted to use thousands of tons per year, then the command should contain `fluxUnit=6`. Flux units should be ones that are customary for the audience and also selected so that they don't require too many digits to be printed on the y-axis scale. The argument `fluxMax` is the upper bound for the y-axis of the graph. If the argument is left out, then the graph is self-scaled. The value for `fluxMax` is expressed in the units specified by `fluxUnit`.

Both of these graphics will have titles that indicate: the name of the site, the water quality variable being plotted, the PA being used (e.g. water year, or season defined by the months of April, May, and June), and designation of what is being plotted. If `blankTime` has been used, then there will be no points plotted for the missing years, and the flow-normalized curve will have a break during the

period of missing data. Examples of these two types of plots are seen in Figure 28 and Figure 29. The commands that produced these figures are `plotConcHist()` and `plotFluxHist(fluxUnit=8)` respectively.

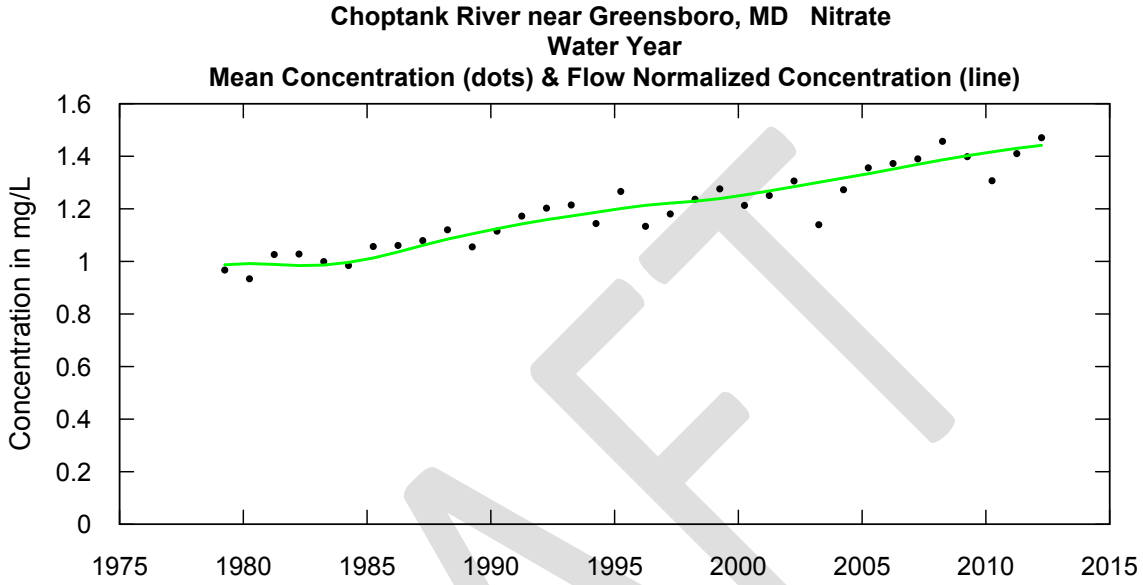


Figure 28. Concentration history graphic produced by plotConcHist function. Choptank River, MD, nitrate data.

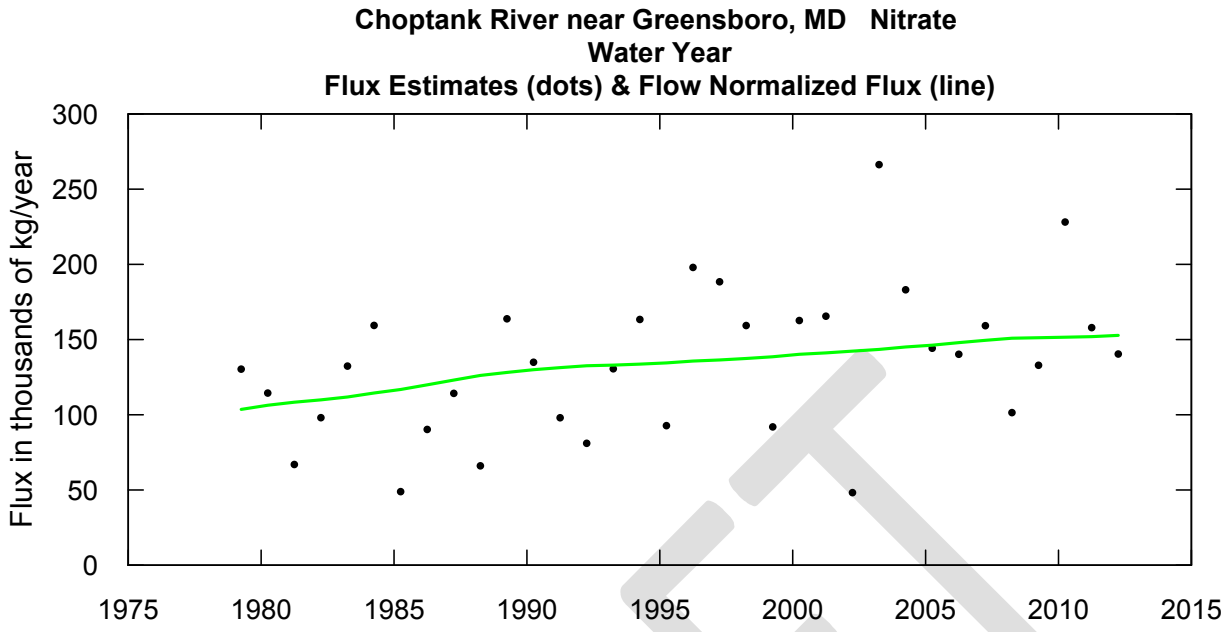


Figure 29. Flux history graphic produced by plotFluxHist function. Choptank River, MD, nitrate data.

For graphics in a report on multiple sites or for multiple constituents it may be desirable for the plots to all start and end at the same date. Setting `yearStart` and `yearEnd` to the same value in all cases will accomplish this. Note, however, that if this is done, the water quality and discharge data from before and/or after the period specified for the graphic will have some effect on the results even though these periods are not shown in the graph. Thus, if the goal is to use the same period of record at all sites or for all constituents, then the records used should be edited down to the desired period before running `modelEstimation`. The process for limiting the length of the data set is described below in the section on editing the data. If the user simply wants to show the results for the entire period of record for the site and constituent of interest, then the two arguments (`yearStart` and `yearEnd`) can simply be left out of the command and the limits of the x-axis will be set automatically by the data.

Producing tables of results

Users may want to publish a printed table of some or all of the results at an annual time step. The function that produces such a table is `tableResults`. It can be used to produce a table that is simply printed to the console, from which the user can copy it and place it into a document, but it can also return a data frame, which has all the necessary information to produce a table suitable for entry into a spreadsheet or a word processing document for publication. The process of producing a table in Excel is described in Appendix B, section 11 (Creating tables in Microsoft from R). The output of `tableResults` has the following columns: year, mean discharge, annual mean estimated concentration, annual mean estimated flux, annual mean flow-normalized concentration, and annual mean flow-normalized flux. The user can select the units for discharge using the `qUnit` argument (default is `qUnit=2`, which is m^3/s) and the units for flux using the `fluxUnit` argument (default is `fluxUnit=9`, which is 10^6 kg/year). If a data frame designed for preparing a publication quality table is desired then the argument `returnDataFrame` should be set to TRUE. Here are two examples of the command.

```
tableResults(qUnit = 3,fluxUnit = 6)
```

In this case the user wants the discharge in 10^3 ft^3/s and flux in 10^3 tons/year with no data frame returned. If the data frame is desired, then the command might look like this:

```
resultsTable <- tableResults(returnDataFrame = TRUE)
```

In this case the user wants the default units (m^3/s) and 10^6 kg/year and wants a data frame returned, with the name `resultsTable`. Figure 30 is an example of output for:

```
tableResults(qUnit = 3, fluxUnit = 6)
```

```
Potomac River at Washington, DC
   Atrazine
   Water Year

   Year    Discharge     Conc     FN_Conc      Flux     FN_Flux
           10^3 cfs           mg/L             10^3 tons/yr
```

```
    1995      8.08    0.1381    0.1368     1.435      1.72
    1996     23.76    0.1770    0.1207     4.193      1.56
    1997     14.44    0.0935    0.1062     0.954      1.38
    1998     20.04    0.0932    0.0958     1.443      1.27
    1999      5.08    0.0716    0.0867     0.289      1.17
    2000      8.34    0.0745    0.0796     0.582      1.10
    2001      7.69    0.0697    0.0746     0.568      1.05
    2002      4.02    0.0592    0.0711     0.346      1.03
    2003     22.83    0.1111    0.0688     3.493      1.02
    2004     17.75    0.0704    0.0672     1.069      1.02
    2005     12.16    0.0605    0.0666     0.658      1.03
    2006      8.74    0.0643    0.0668     0.919      1.07
    2007     10.50    0.0481    0.0675     0.479      1.11
    2008     10.44    0.0704    0.0693     1.426      1.18
    2009      8.89    0.0782    0.0728     1.387      1.29
    2010     13.06    0.0523    0.0778     0.607      1.42
NULL
```

Figure 30. Example output from `tableResults`, for Potomac River at Washington, DC, Atrazine data.

Computing and displaying tables of change over time

The function `tableChange` provides measures of change, in both flow-normalized concentrations and in flow-normalized flux, between pairs of years selected by the user. The function computes a total of eight change measures for any given pair of years. For flow-normalized concentrations these are: change in flow-normalized concentration expressed in mg/L, the slope of flow-normalized concentration change expressed in mg/L per year, the change in flow-normalized concentration in percent, and the slope of the flow-normalized concentration change in percent per year. For flux, the user specifies the units to use to measure flux (the default units are 10^6 kg/yr). The change measures are respectively: the change in flow-normalized flux, the slope of the change in the flow-normalized flux in flux units per year (e.g. 10^6 kg/yr/yr), the change in the flow-normalized flux in percent, and finally the slope of the change of the flow-normalized flux in percent per year. The command is:

```
tableChange(fluxUnit, yearPoints)
```

The object `yearPoints` is a vector of integer numbers, in ascending order, which is the full set of years for which the user wants to make comparisons. This is best explained by an example. If one wanted to examine the changes between 1996 and 2003 and between 2003 and 2010, then `yearPoints` would be specified as:

```
yearPoints <- c(1996,2003,2010)
```

That indicates that the full set of comparisons (changes or slopes) that will be made are all of the possible ordered pairs of these years. If the requested set of `yearPoints` exceeds the actual data, the `tableChange` output reverts to a default set made up of 5-year increments and multiples of 5-year increments. In the case considered in this example, those ordered pairs are: 1996-2003, 1996-2010, and 2003-2010. Having defined `yearPoints` as shown above the command for quantifying the changes using flux units of 10^3 tons/year is:

```
tableChange(fluxUnit=6, yearPoints)
```

Or this could be done in a single command line as:

```
tableChange(fluxUnit=6, yearPoints=c(1996,2003,2010))
```

The output for this command is shown in Figure 31.

```
  Potomac River at Washington, DC
  Atrazine
  Water Year

          Concentration trends
  time span       change     slope    change     slope
                    mg/L   mg/L/yr         %       %/yr

1996  to  2003    -0.052   -0.0074       -43       -6.1
1996  to  2010    -0.043   -0.0031       -36       -2.5
2003  to  2010     0.009    0.0013        13        1.9


                Flux Trends
  time span          change         slope       change         slope
                 10^3 tons/yr   10^3 tons/yr /yr      %           %/yr
1996  to  2003         -0.55       -0.078          -35           -5
1996  to  2010         -0.14        -0.01         -9.3        -0.66
2003  to  2010           0.4        0.057           40          5.6
```

Figure 31. Output from `tableChange` function for Potomac River at Washington DC, Atrazine.

There is an alternative version of the function `tableChange`, called `tableChangeSingle`, which creates a data frame that contains the contents of the table. The arguments are the same as in `tableChange`, except that there are two additional logical arguments `returnDataFrame` and `flux`. If a data frame is going to be returned then the command to produce only the concentration output portion of Figure 31 would be:

```
changeTableConc <- tableChangeSingle(yearPoints, returnDataFrame=TRUE)
```

To return only the flux results, the command would be:

```
changeTableFlux <- tableChangeSingle(fluxUnit=6, yearPoints,
returnDataFrame=TRUE, flux=TRUE)
```

These two data frames, `changeTableConc` and `changeTableFlux`, can be written to files and be used to create Excel spreadsheets for use in a report (see Appendix B section 11).

A wide range of change measures are presented in the output of these functions in order to facilitate a variety of comparisons across constituents, sites, and time frames. In addition to comparing rates of change over various time periods, another comparison that is particularly worthy of note is the comparison, for the same time period, of changes in flow-normalized concentration expressed in percent versus changes in flow-normalized flux expressed in percent. If the nature of the change in the system were such that the trend in the log of concentration was the same across the full range of discharges and the full range of seasons, then it is mathematically assured that the change in percent for flow-normalized concentration and flow-normalized flux would be equal to each other. Using the LOADEST model this equality must hold true because it assumes that the trend in the log of concentration is the same across all discharges and across all seasons. In the example shown in Figure 31 this is far from the case. The flow-normalized concentration change from 1993-2010 is estimated to be 13 percent but the flow-normalized flux change over that same period is estimated to be 40 percent. What this means is

that the change (in percentage terms) in concentration over this period of time is greater for high discharges than it is for low discharges.

It is entirely possible for the changes in flow-normalized concentration to be of the opposite sign from changes in flow-normalized flux. If, for example, there were large decreases in point source inputs of a pollutant but increases in non-point sources associated with high flow events then we would expect to see a negative trend in concentration but a positive trend in flux. For example, the total Phosphorus record for the Susquehanna River at Conowingo Maryland (Hirsch, 2012) shows that over the period 1982-2012 the change in flow-normalized concentration was a decrease of 17 percent, but the change in flow-normalized flux was an increase of 13 percent. The explanation for this apparent anomaly is that the monitoring site is located at Conowingo Dam, just upstream of the Chesapeake Bay. This dam is rapidly becoming full of sediment and with it a great deal of phosphorus attached to those sediments. In recent years, high flow events have delivered much higher fluxes of total phosphorus past the dam than they would have in previous years, because the reservoir's ability to store the sediment entering from upstream is greatly diminished from what it had been and the tendency for scour of reservoir sediment has increased. These two factors contribute to a substantial increase in flux. However, at the same time, substantial efforts are ongoing upstream of the reservoir to limit phosphorus inputs from the Susquehanna River Basin, and concentrations of total phosphorus entering and exiting the reservoir at moderate to low flow conditions have been declining. Because these improvements manifest themselves over a large fraction of the time, they lead to decreases in average concentrations in the water going past the dam, even though concentrations on the few highest flow days have been increasing. Thus, investigations of trends in concentration may not be informative at all about trends in flux. It is useful to recall that statements about average concentrations are really statements about concentrations integrated over time, but statements about average fluxes are really statements about the

product of concentration and discharge integrated over time, and thus the days of the highest discharge can strongly influence flux trends and have little influence on concentration trends. An important attribute of the WRTDS method is that it allows for examination of both concentration and flux, and does so within the same computational framework. These diverse kinds of changes, revealed by these comparisons of percentage changes in concentrations and flux, can be further explored using some of the tools introduced in the later section on "Exploring model behavior and adjusting model parameters".

Exploring the quality of the fitted model - overview

Even though the WRTDS model is highly flexible, there is no assurance that it will provide reasonable estimates of concentration and flux for all days in a record. The graphical tools can help identify serious problems with the model fit. The EGRET package makes it easy to produce and view a large number of these graphics quickly. Many of these graphics are types of residuals plots, in which the model residuals (observed minus predicted values of log(*c*)) are plotted against predicted values or against other explanatory variables. The following is a list of the types of problems that these graphics can help identify.

- One of the problems that can arise with models such as WRTDS or LOADEST is a tendency toward severe under-prediction or over-prediction of concentrations on days of particularly high discharge. This can happen because the data at the highest discharges may be sparse and the model may not be sufficiently flexible to capture the particular curvature that exists in the ln(c) versus ln(Q) relationship. When this happens it can result in severe under-prediction or over-prediction of annual or long-term mean fluxes.
- Another problem is the possibility that concentrations are severely under-predicted or over-predicted for a period of many months to years. This can arise particularly in large watersheds where there can be long periods when the discharge is disproportionately derived from one

portion of the watershed that may be source of water with particularly high or particularly low concentrations. This can have a serious impact on annual or seasonal estimates of concentration or flux but is unlikely to have much of an influence on long-term mean flow-normalized values.

- Yet another type of problem that can arise is when the changing conditions of the watershed are dominated by abrupt changes in one particular point source. WRTDS makes an implicit assumption that changes in the system are gradual and typically a result of an aggregate of many actions taking place at different times: for example many small changes in point source loadings, gradual shifts in land cover or in land use practices across the entire watershed, gradual adoption of management practices by many land-owners; or changes in farming practices or urban landscape modifications. There are certainly situations where a major cause of water quality change is an enhancement of a single large point source discharge. Plots of residuals versus time can help identify situations where this may be happening and can be used to design alternative methods to properly model what is happening (including downward adjustment of the `windowY` parameter).
- Finally, there are cases where the seasonality of the system is very strong and the changes between seasons are very abrupt. In such cases the smooth representation of seasonality that WRTDS produces may not capture this pattern very well although downward adjustment of the `windowS` parameter may help improve these results.

To facilitate rapid exploration of serious problems with WRTDS models, the EGRET software has a single function that produces a set of eight diagnostic graphics on a single page. This function is called `fluxBiasMulti`. It is described in more detail below. The graphic it produces is designed to help the hydrologist quickly spot potential problems. Any one of the eight graphics in the plot can be produced individually in a larger graphic that would be suitable for publication or presentations.

Flux bias statistic

In the `fluxBiasMulti` function the resulting graphic includes the flux bias statistic. This statistic was created in response to a problem that several authors have identified regarding some of the more common methods for estimating average annual and long-term mean fluxes. This problem was first described by Stenback and others (2011) and that paper introduced the use of a statistic that is the functional equivalent of the flux bias statistic used here. Subsequently, others have described and explored this problem, notably Garrett (2012), Moyer and others (2012), Richards and others (2012), and (Hirsch, In Press). Most of the discussion in these papers has been about the use of the LOADEST model (first developed by Cohn and others (1992) and subsequently published in the LOADEST software package (Runkel and others, 2004)). The LOADEST model is a regression-based method which uses either the same equation as WRTDS (equation 6) or one that also adds quadratic terms in ln(Q) and in time. LOADEST, unlike WRTDS, uses a single set of parameters to describe the relationship of ln(c) to discharge, time and season rather than using locally weighted regression like WRTDS. The motivation for development of the flux bias statistic was to use it as an indicator of possible flux bias in LOADEST models, but it can be used to explore flux bias in WRTDS models as well.

The flux bias statistic as defined here is a dimensionless representation of the difference between the sum of the estimated fluxes on all sampled days (P) and the sum of the true fluxes on all sampled days (O).

$$B = (P - O)/P \text{ where:} \tag{10}$$

$$O = \sum_{i=1}^{n} L_i = \sum_{i=1}^{n} k \bullet c_i \bullet Q_i \tag{11}$$

$$P = \sum_{i=1}^{n} \hat{L}_i = \sum_{i=1}^{n} k \bullet \hat{c}_i \bullet Q_i \quad (12)$$

Where

L_i is the observed load on the i[th] sampled day in kg/day

$\hat{L}_i$ is the estimated load on the i[th] sampled day in kg/day

k is a units conversion factor = 86.4

c_i is the measured concentration on the i[th] sampled day (in mg/L)

$\hat{c}_i$ is the estimated concentration on the i[th] sampled day, it is a "leave-one-out cross validation estimate" as discussed above in the section on the `modelEstimation` function

Q_i is the discharge on the i[th] sampled day (in m^3/s)

and

n is the number of sampled days

A value of *B* near zero suggests that the model is nearly unbiased. Positive value suggests a positive bias, and a negative value suggests a negative bias. Values of *B* that are between -0.1 and +0.1 indicate that the bias in estimates of the long-term mean flux is likely to be less than 10 percent. In a study (Hirsch, In Press) where true flux can be well estimated (because sampling frequencies are very high) it has been shown that the relationship between the true bias and the B statistic is highly non-linear and is rather imprecise. The flux bias statistic is not a basis for making corrections in flux estimates, but it can identify cases that are likely to have severe biases, which should motivate the hydrologist to seek some means to resolve that problem by use of a better statistical model. The work of Moyer and others(2012) and (Hirsch, In Press) indicates that WRTDS is substantially less prone to severe flux bias, but it is not immune to the problem. The flux bias statistic, shown on the `fluxBiasMulti` output, is one more tool that can help identify problematic situations where model

parameters need to be adjusted or where the WRTDS model may simply not be suitable for application. Hirsch, (In Press) identified three common causes of severe flux bias, 1) a model that is poorly suited to the true relationship between ln(c) and ln(Q), 2) substantial seasonal differences in the shape or slope of the ln(c) versus ln(Q) relationship that are not accounted for by the model, and 3) substantial heteroscedasticity of model residuals. Identifying these three problems were the primary motivations behind the development of this set of graphics.

Graphics for examining the quality of the model

As a general rule, before any regression-based model is used the hydrologist should carry out some graphical checks to determine if there are serious departures from the model assumptions, and then consider changing the model estimation method to account for those departures. The WRTDS model is designed to be highly flexible (i.e. the assumptions it uses are less restrictive than other regression-based methods) it is still important to graphically evaluate the adequacy of the fitted model. The diagnostic tools shown here can be very useful in evaluating the appropriateness of such models. The design of the EGRET software makes it possible to check the adequacy of other models and compare them to WRTDS. This can this can be done by creating alternative versions of the `Sample` and `Daily` data frames that contain the estimates from those alternative models. This is described in the section "Working with multiple versions of data frames".

The examples presented here come from a data set of 240 observations taken over a 10-year period for nitrate for the Vermilion River, at Pontiac, IL. The watershed is 1500 km^2 at this location and is dominantly agricultural. There are 8 different graphics that are combined into a single graphic using the function `fluxBiasMulti` shown in Figure 32. Each of these 8 graphics can be used to produce a standalone figure, more details about these standalone functions can be found in Appendix B or the individual help pages for these functions. An additional graphic is shown in Figure 33 which is based

on the same data set, but it was fitted with the half-window widths of the WRTDS model set to very high values (`windowY = 100, windowQ = 10, and windowS = 10`). By setting the half-window widths to such large values, the weights on all of the observations in each of the regressions become virtually equal. The consequence of this is that the model becomes essentially a non-weighted regression of the log of concentration on time, log discharge and sine and cosine of time of year. This is virtually identical to the LOADEST 5-parameter model which has often been used to fit these kinds of data sets to for evaluation of fluxes and long-term water quality trends. Several of the component graphics of Figure 33 show some of the consequences that can arise from using an inappropriate model.

The arguments used in `fluxBiasMulti` that produced Figure 32 are these (shown here with their default values): `qUnit = 2, fluxUnit = 3`, and `moreTitle = "WRTDS"`. The arguments `qUnit` and `fluxUnit` have been introduced in the section "Summarizing Water Quality Data (without using WRTDS)". The argument `moreTitle` allows the user to provide a name to the graphic that will help to identify it in cases where multiple models are being considered. The default is `"WRTDS"` which simply causes "WRTDS" to be printed as a part of the graphic's title, but any string of characters, enclosed in quotes, can be used here to identify the model, for example "approx LOADEST 5" used in Figure 33. In the particular case shown here, the graphic in Figure 32 was sent to a pdf of a particular size, to assure the best possible formatting, although even without this formatting the graphic is quite useable for purposes of identifying model errors. The set of three commands used here were:

```
pdf("fluxBiasMultiVermNO3.pdf", height = 9, width = 8)
fluxBiasMulti(fluxUnit=4)
dev.off()
```

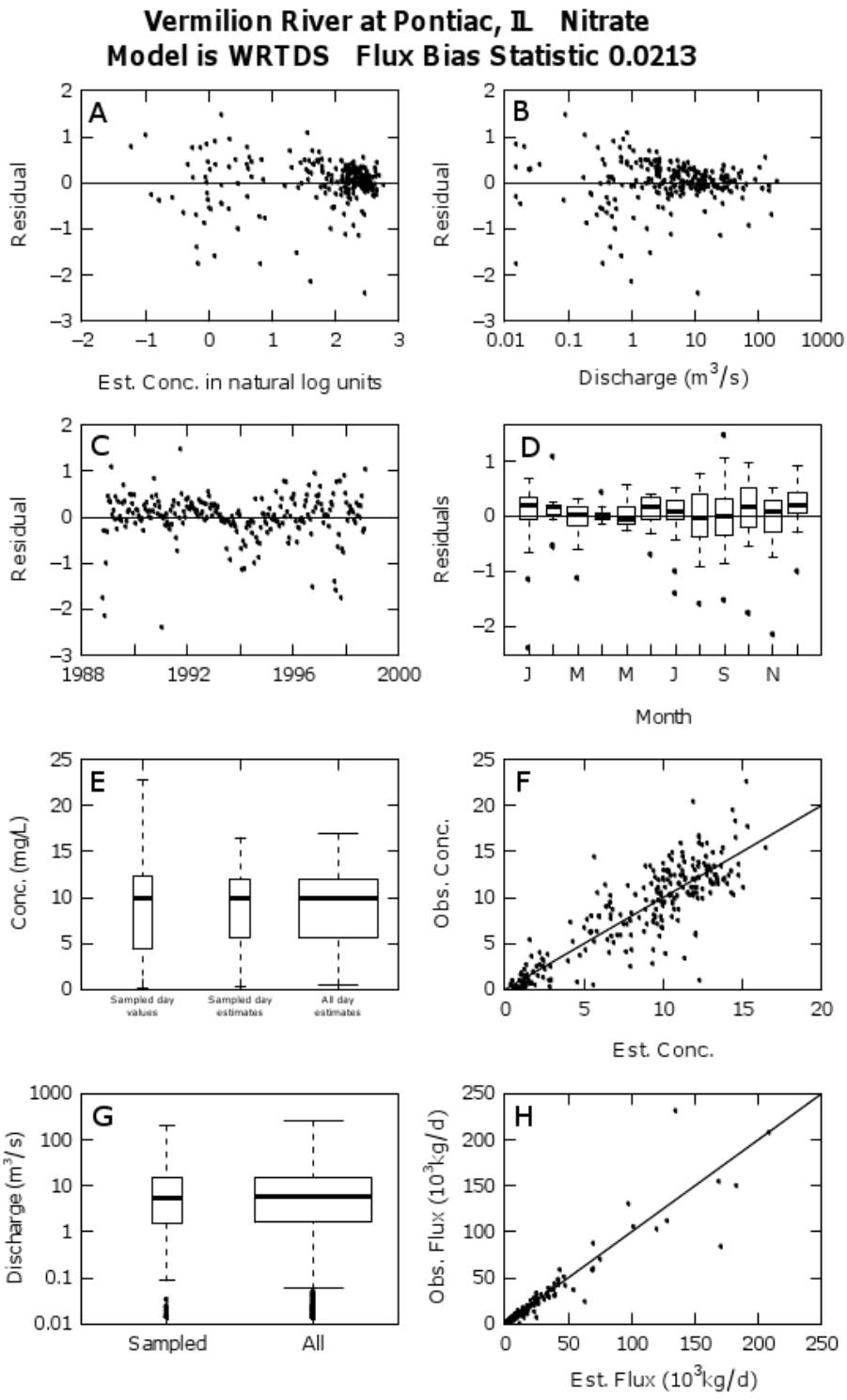

Vermilion River at Pontiac, IL Nitrate
Model is WRTDS Flux Bias Statistic 0.0213
A
Residual
Est. Conc. in natural log units
B
Residual
Discharge (m3/s)
C
Residual
D
Residuals
J M M J S N
Month
E
Conc. (mg/L)
Sampled day values
Sampled day estimates
All day estimates
F
Obs. Conc.
Est. Conc.
G
Discharge (m3/s)
Sampled
All
H
Obs. Flux (10^3kg/d)
Est. Flux (10^3kg/d)

Figure 32. Output of fluxBiasMulti function for Nitrate for the Vermilion River at Pontiac, IL. Description of each of the 8 panels is presented in the text of the report.

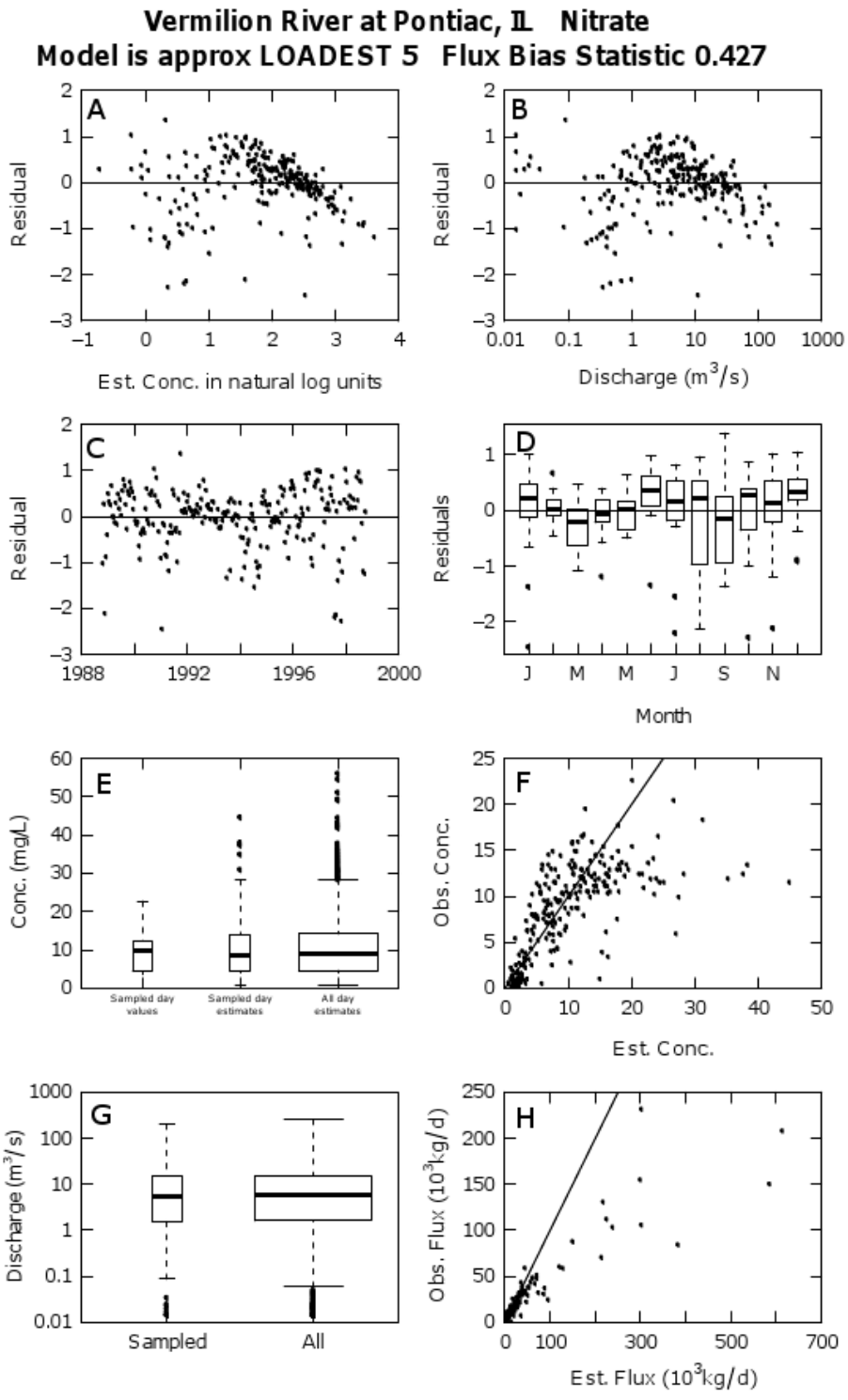


Figure 33. Output of fluxBiasMulti function for Nitrate, Vermilion River at Pontiac, IL using a model approximating LOADEST 5.

This string of commands causes the graphics file to have the name `fluxBiasMultiVermNO3.pdf` to be created and have a height of 9 inches and a width of 8 inches. The component parts of the graphic are these:

A. `plotResidPred` produces a graph of the residuals of the WRTDS model as a function of the model estimates. Both the residuals and the model estimates are in the natural log concentration units in which the model is fitted. The features of this graphic that are of interest are the degree of symmetry of the residuals around the zero line and the presence of curvature. Lack of symmetry would suggest that the errors of the WRTDS model depart from normality. Over many applications of WRTDS it has generally been found that modest amounts of asymmetry or departures from normality are generally not sufficiently important to require corrective steps be taken. Curvature is generally not a serious problem unless the smoothing window widths are much too wide for the range a values of the explanatory variables. The version of this graphic for "approx. LOADEST 5" shows a substantial amount of curvature. Of particular note is the fact that for estimates of log concentration greater than about 3, the residuals are all negative, indicating that the model greatly over-predicts concentration. Also, in a middle range of estimates, from about 1 to 2 log units, almost all residuals are positive, meaning that the model greatly under-predicts in this range.

B. `plotResidQ` produces a graph of the residuals of the WRTDS model as a function of the log of discharge. In general, this figure will look rather similar to the previous one, because discharge is often the single most important determinant of concentration in the WRTDS model. In this case there is no apparent lack of symmetry or curvature that would suggest that the model is inappropriate. One feature that is particularly noteworthy here is that the variability of the residuals appears to be smaller at high discharges than at low discharges. This does not present a problem for the WRTDS model, because the variability is estimated for each observation or estimation point and

the bias correction is determined based on that estimate of variability. Some of the standard regression-based models (such as LOADEST) require an assumption of homoscedastic residuals and even if those models properly dealt with the curvature of the data, they would not produce reasonable bias correction factors. The graphic on Figure 33 shows again the strong curvature of the relationship with almost all estimates for discharge values greater than about 50 m^3/s being too high (negative residuals). There is a particularly complex pattern of residuals at the lower discharge values showing positive residuals for discharges around 0.02 m^3/s, and negative residuals between about 0.1 and 1 m^3/s. This pattern suggests that the model used to fit these data is highly flawed.

C. `plotResidTime` produces a graph of the WRTDS residuals as a function of `DecYear`. There are two specific issues that this type of figure might suggest, beyond what the two previous ones might reveal. One is the possibility of a sudden step change at some point in time. Because WRTDS is fundamentally a smoothing algorithm, it is best suited to a situation where changes are gradual. For example the changes may come from gradual adoption of new land use management practices across many landowners and communities in a watershed, or the combination of a number of improvements in point-source controls, each one happening at a different time. But there are certainly cases where a single event has a profound effect on water quality in a watershed. This might be the completion of a major upgrade of a large waste treatment facility, or a major change in the routing of wastewater or storm water in a basin, perhaps through an interceptor sewer and into a different watershed or into a new holding facility for storm water. If a step function is indicated in this plot then that is an argument for doing other kinds of analyses that treat conditions before the change as a different population from those after the change, and to then evaluate the magnitude and nature of this shift. This might be done by creating two WRTDS models one for the period before the shift and one for the period after the shift and comparing their behaviors. The other issue of

interest that the `plotResidTime` graph may reveal is a relatively long period of dominantly negative or dominantly positive residuals. This can suggest that there are processes at work in the watershed that deliver significantly different types of water to the monitoring location. One possible cause for this can be found in very large watersheds, where in one particular year a large fraction of the flow comes from one sub-watershed while in other years that same sub-watershed supplies a small fraction of the flow. This kind of situation has been observed in the case of nitrate in the Missouri River (see discussion by Kahlkoff, (2013)) during the flood of 2011. The source of this flood was heavy precipitation in the upper Missouri Basin, which has much lower nitrate concentrations than are produced from tributaries in the lower basin, which has been the source of most of the water in other recent flood events. As a consequence nitrate concentrations during this multi-month flood were all much lower than would be predicted by the WRTDS model. The results for the Vermillion River shown in Figure 32 indicate that from the spring of 1993 through the fall of 1994 there was a long period of negative residuals. This departure started with the beginning of the extreme high flows of the 1993 flood (that affected most of the upper Mississippi River Basin including the Vermilion River) and continued until well after the conclusion of that event. This is a common type of occurrence, that prolonged high flows can result in a subsequent period of negative residuals, indicating that solute flux is lower than what would be expected based on discharge and time of year, because the large high flow event had the effect of flushing the watershed of a significant part of its stored nitrate. The opposite condition is also true of low flow events. High flows that follow long and severe low flows can have dominantly positive residuals, because of the amount of solute that remains in storage in the watershed. This topic has been explored further in (Murphy and others, 2014). These kinds of long-term departures from residuals of approximately zero mean suggest that the error process is far from independent and that estimates for individual years could

be improved by explicit use of the information seen in these residual time series. Development of enhancements of WRTDS to account for this kind of persistence is a high-priority topic for further model development.

D. `boxResidMonth` produces a graphic of the WRTDS residuals as boxplots by month. In the ideal case these boxes should all be approximately symmetrical around a value of zero. Substantial positive or negative departures for several months can indicate that the model is not fully accounting for real seasonal differences in system behavior. There is some indication of this in Figure 32 showing that residuals have a tendency to be positive particularly in the months of June, July October, December, January and February. The fact that these are spread across a wide range of months suggests that there is not a simple explanation for this departure and that there is no simple fix for it. In some cases, with large data sets, the use of a narrower seasonal window width (`windowS`) might be able to reduce some of this seasonal bias (it was not found to be useful in this case). Figure 33 shows a similar and somewhat stronger pattern, suggesting that the model approximating LOADEST-5 has less ability to fit the seasonal pattern than the WRTDS model does.

E. `boxConcThree` produces a graph containing three boxplots of concentration. The first is a boxplot of the measured concentration values (`Sample$ConcAve`). The second is a boxplot of the WRTDS model estimates of concentration for all of the days on which there were measurements (`Sample$ConcHat`). As described previously, these are cross-validation estimates, and as such they are computed without the knowledge of the actual concentration on the day for which they are estimated. The third boxplot is for the WRTDS estimates of concentration on all days in the period of record (`Daily$ConcDay`). The width of each of these boxplots is proportional to the square root of the sample size, thus the third box is substantially wider than the first two. The example shown in Figure 32 is a good example of what we would expect to find for a model that is performing

properly. In particular, the medians for all three sets are virtually identical and the overall shapes of the distributions are similar in terms of the median and interquartile ranges. The distribution of actual sample values does show slightly more variability than the other two, in terms of the interquartile range and particularly the extreme values. This is exactly what should be expected. Estimates based on regression methods which fit the data reasonably well (such as WRTDS) will always show less variability than is seen in the sample data on which they are based. Estimates will always "regress to the mean." The fact that the second and third boxes are quite similar to each other is an indication that the set of sampled days covers a range of values of the explanatory variables that is similar to the range of values in the full set of days in the period of record. If the number of sampled days is rather small, or fails to cover a large part of the range of values for the full record, then the third box may show somewhat more variability than the second. However, when there are serious problems with the model fit, as shown in Figure 33 it is common for the extreme values of the sampled day estimates and of all daily estimates to be much greater than the extremes observed in the sample data. For example, in this case, the maximum sample value is 22.7 mg/L, the maximum estimate on a sampled day is 44.9 mg/L, and the maximum estimate on all days is 56.4 mg/L (in the WRTDS case the latter two were 16.5 mg/L and 16.9 mg/L respectively). High values of the daily estimates, which vastly exceed the high values in the original sample, are a very strong indicator that a model is seriously flawed. This plot provides a very simple way to make the necessary comparisons.

F. `plotConcPred` produces a scatter plot of observed concentration values (`Sample$ConcAve`) as a function of the estimates for those days (`Sample$ConcHat`). It also shows a 1:1 line. A model that fits well should be tightly clustered around that 1:1 line and should generally be roughly symmetrical around that line. Average departures above the line should roughly balance departures

below the line. This example shows some large departures from the 1:1 line, and some tendency towards underestimates when the estimated values are in the vicinity of 15 mg/L but conversely, some tendency towards large overestimates when the estimated values are between about 8 and 12 mg/L. It shows that errors can be large, but there does not appear to be a strong tendency towards bias in one direction or the other. In Figure 33 this panel provides another representation of the problem illustrated in the differences between the first two boxes in `boxConcThree`. It shows that estimates higher than about 20 mg/L are typically extreme overestimates, that can be anywhere from 5 to 30 mg/L higher than their true values. Conversely, for estimates between about 5 mg/L and 15 mg/L there is a strong tendency for the model to produce underestimates of up to about 5 mg/L but overestimates are infrequent and small. This graph is somewhat similar to what is shown in the `plotResidPred` graph (panel A of these two figures), the difference being that these are shown in real concentration units and also that the bias correction factor has been applied here. Note that the residuals in panels A through D are all the residuals in the log of concentration and no bias correction is involved in computing these values. In contrast, panels F, G, and H all consider estimates of concentration or flux and the computation of these values do involve use of the bias correction factor. Thus, these `plotConcPred` graphs show the compound effects of inadequate model fit and issues related to heteroscedasticity and its influence on the bias correction.

G. `boxQTwice` produces a pair of boxplots of discharge, on a log scale. This graphic also appears in the output of `multiPlotDataOverview`. The first box represents the log discharge values on all sampled days (`Sample$LogQ`). The second box represents the discharge values on all days in the period of record (`Daily$LogQ`). The box plots are produced in the log units, which are then plotted against a logarithmic discharge scale (rather than being developed from the raw discharge data). These plots do not contain any information about the concentration data or the quality of the fit, but

they are very useful indicators of the distribution of discharges in the sample data set. What would be particularly disturbing would be the case where the first box was shifted downwards in relationship to the second box. This would indicate a pattern of under-sampling the higher discharges, which are often the most important to quantify and this would be problematic for studies focused on the estimation of flux or trend in flux. Sampling schemes that preferentially sample at the higher discharges, but still cover much of the range of discharge values, have been shown to generally produce better estimates of flux than those that approximate a random sample of discharge values see (Hirsch, In Press). In this particular case the two boxes are very nearly equivalent which should come as no surprise, because the sample values are a random sample from a virtually complete daily data set.

H. `plotFluxPred` produces a scatter plot showing observed flux values on all sampled days (`Sample$ConcAve*Sample$Q*86.4`) as a function of estimated flux values on all sampled days (`Sample$ConcHat*Sample$Q*86.4`). It also shows a 1:1 line. The plot is designed to provide a graphical representation of potential bias in flux estimates. A biased model would show substantial asymmetry in the distribution of departures above and below the 1:1 line. In the case shown in Figure 33, the results are excellent and this is well reflected in the flux bias statistic shown at the top of the figure (0.0213, which represents an average error of +2.13 percent). In Figure 33 the estimates depart substantially from the 1:1 line. At the most extreme cases, days with estimated flux values of about $600 \bullet 10^3$ kg/d, the true values were in the range of $150 \bullet 10^3$ kg/d to $200 \bullet 10^3$ kg/d. This strong bias is reflected in the flux bias statistic 0.427 shown at the top of Figure 33 (an average error of +42.7%).

There are two additional graphical functions that can be useful to understanding quality of the model fit. These are `plotConcTimeDaily` and `plotFluxTimeDaily`. Both of these functions operate in the same manner and this discussion will focus on `plotConcTimeDaily`. This function produces a graph of the daily estimates of concentration as a function of time (`Daily$ConcDay` as a function of `Daily$DecYear`), which is shown as a continuous line and also a set of points that represent the observed values of concentration as a function of time (`Sample$ConcAve` as a function of `Sample$DecYear`). Figure 34 is an example of a three-year segment for the same data and model shown in Figure 32.

The default command for this function is just `plotConcTimeDaily()` and this will produce a plot for the entire period of the `Daily` data frame. In general, these will be somewhat difficult to interpret because they can be dominated by the very steep rise and fall of the curve of estimated values. Making such a plot can help to identify time periods within the record that may reveal interesting patterns. Once these periods have been identified a revised version of the graphic can be produced, focusing on a short portion of the period of record. The first two arguments to `plotConcTimeDaily` define the start and end of the time period to be plotted: `startYear` and `endYear`. Figure 34 was produced by the following command `plotConcTimeDaily(startYear = 1992, endYear = 1995)` or equivalently `plotConcTimeDaily(1992, 1995)`.

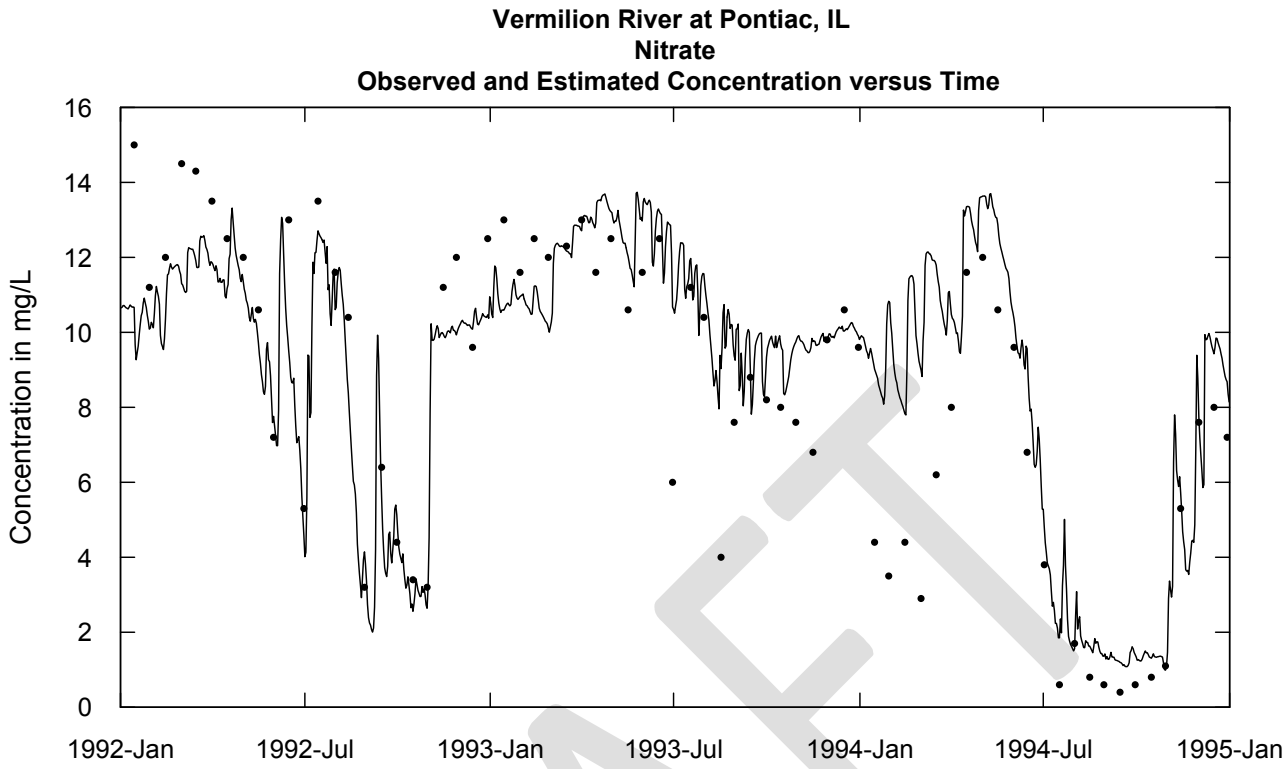


Figure 34. Output of plotConcTimeDaily for the years 1992-1994, for the WRTDS model of nitrate for the Vermilion River at Pontiac, IL.

There are several features of this figure that are notable. For this period of the record, the model starts by doing rather poorly at estimating the very high values observed in the winter and early spring of 1992, then the model does well in capturing alternating high and low concentration values through much of the rest of 1992 and the prolonged period of relatively high values during the winter and spring of 1993. However, it does poorly at estimating concentrations during parts of the very high flow period of 1993 (summer) and very poorly in the winter and spring of 1994 (in the aftermath of the large flood) substantially overestimating concentrations during this period. In addition, the model severely overestimates the extremely low concentrations values in the late summer and early fall of 1994. This

figure is a reminder that although the model fitted here has rather good properties in terms of overall fit and has a low flux bias, there can be extended period for which it produces estimates that are either substantially too high or too low. There are important processes that influence concentration that this simple statistical representation does not capture, but doing the WRTDS analysis helps the user gain understanding of the system by removing the variability that can be explained by time, discharge and season, thereby revealing the remaining variability. This kind of observation, of sustained over-estimates or under-estimates, can be an excellent point of departure for more detailed exploration of the factors that may be driving water quality at this location. This can be seen to some extent in panel C of Fig 32 and 33 but figure 34, with its higher temporal resolution, may provide more insight about this behavior.

Figure 35 is a representation of the model estimates produced by the model used in Figure 33 (the approximation of the LOADEST 5 model). Note that the vertical axis now runs from 1 to 40 mg/L versus the Figure 34 where it only ran from 0 to 16 mg/L. As the previous diagnostic plots suggest, this model makes very large overestimates of concentration particularly during the very wet spring of 1993 as well the winter and spring of 1994. It also seriously overestimates the very low concentrations in the summer of 1994 although it makes quite reasonable estimates during the late summer and fall of 1992 and 1993. In short, it shows concentration estimates that are much too high both at the extreme high flow and extreme low flow conditions.

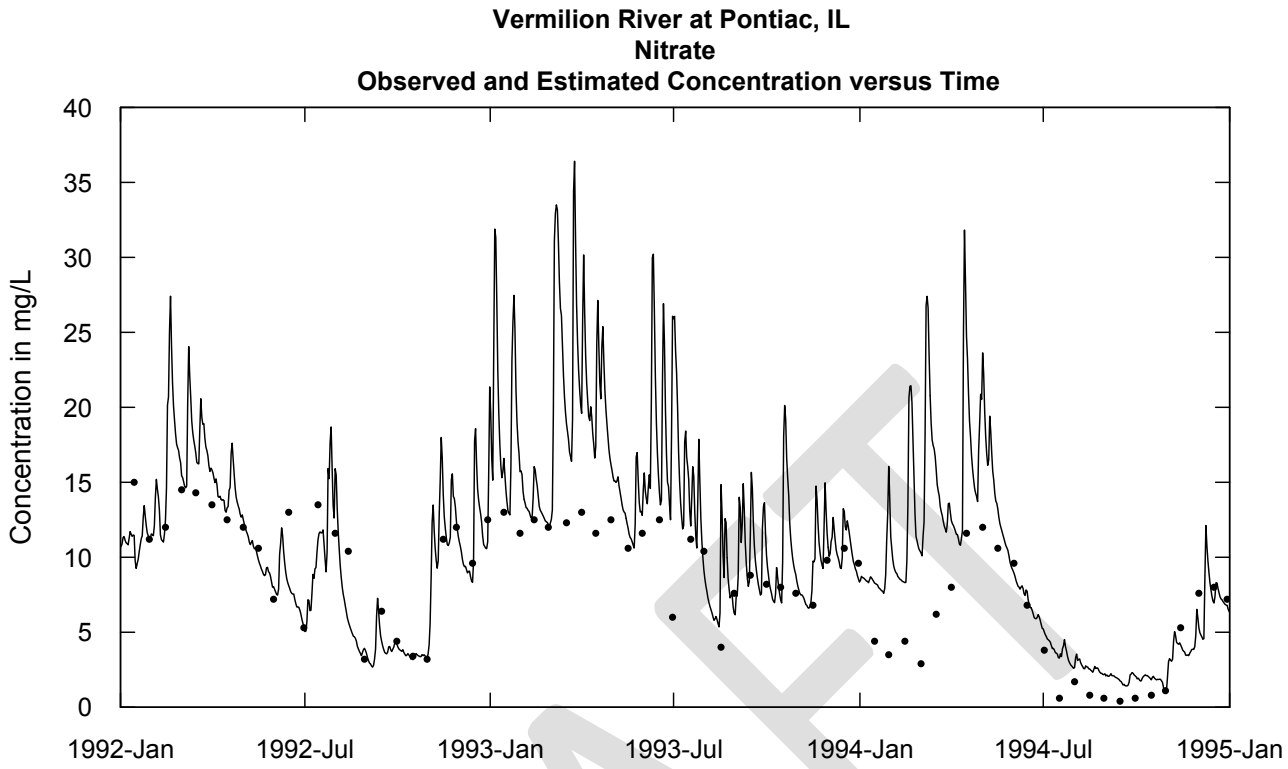


Figure 35. Output of plotConcTimeDaily for the years 1992-1994, for the model that approximates the LOADEST 5 model, for the Vermilion River at Pontiac, IL.

The function `plotFluxTimeDaily` operates in the same manner as `plotConcTimeDaily`. It is often more difficult to assess issues with the model using `plotFluxTimeDaily` because the range of variation in flux is typically so much greater than with concentration. However, it can be useful in gaining a sense of how problems of model fit may influence flux results, which may be the topic of greatest interest in some studies.

Exploring model behavior and adjusting model parameters

plotContours

The idea of contour plots of the three surfaces (`yHat`, `SE`, and `ConcHat`) was introduced in the section "WRTDS analysis of water quality data". They are very central to the WRTDS modeling analysis, because they depict the model's full characterization of the behavior of concentration as a function of time, discharge, and season. This section is designed to provide guidance on how these graphics are generated and how they can be designed to be used effectively, both for exploration being done by the hydrologist and for final presentation of findings.

A description of all of the possible arguments of the `plotContours` function is provided in the function help pages and in the vignettes, but this discussion will focus on the critical arguments that the hydrologist needs to use to obtain a useful result. These key arguments are listed in Table 10. A few basic choices need to be considered in preparing one of these contour plots: setting the discharge range for the plot, deciding if flow duration information will be shown on the plot, setting the time range for the plot, and setting the contour levels. The following paragraphs discuss each of these choices.

The vertical axis of the graphic is a discharge range, determined by the two arguments `qBottom` and `qTop`. These can be set to any values (provided that `qBottom` < `qTop`) but it is best to have their values not extend to the most extreme high and low discharge values in the data set. The concentration estimates shown at the most extreme values of discharge will be much less reliable than those that are located towards the center of the distribution and there will be a tendency for people to over-interpret the information depicted at these extremes. The estimates depicted at these extreme discharges will have very limited influence on the results (such as annual or long-term mean concentrations or fluxes) because they are in a low probability region of the discharge-time domain. Using the `flowDuration` function before setting `qBottom` and `qTop` can be very helpful. A good rule of thumb is to set `qBottom`

to a value close to the 5th percentile on the flow duration curve and set `qTop` to a value close to the 95th percentile on the flow duration curve. Just like `flowDuration`, the `plotContours` function allows to user to select the units for depicting discharge (`qUnit`). The values of `qBottom` and `qTop` are expressed in those units. For the best graphic results, the values of `qBottom` and `qTop` should be integer multiples of 1, 2, or 5 (for example 10, 20, 50, 100, 200 etc.).

One of the options is to have the `plotContours` graphic include a pair of curves superimposed on the plot that have a period of one year and represent seasonally-specific flow duration information. In the default case they are plotted at the 0.05 and 0.95 points on the flow duration curve, which is calculated from the daily flow information using a moving seasonal window. The default width of this window is 60 days either side of the center date. The advantage of plotting this flow duration information is that it indicates which portions of the plot depict relatively rare combinations of discharge and time of year, and which are centered in the mid-range of the flow duration curve. Because the plot is designed as a rectangle, there can be portions of the plot that are based on very limited information (e.g. very high flow in the dry season of the year) but which are also unimportant to the results because they represent conditions that are very rare. The disadvantage of presenting the flow duration information is that it tends to complicate an already complicated and unfamiliar graphic. The hydrologist doing the analysis may want to include these curves to help define the best possible range of discharge values to use in their graphic, but when producing the graphic for presentation purposes, they may chose to leave this information out for the sake of simplicity. The argument for plotting this curve is the logical variable, `flowDuration`. The default value is `TRUE`, meaning that these two curves are shown. A good rule of thumb is to make the vertical scale of the graphic such that the area below the lower curve and above the upper curve are a rather small fraction of total plot area. This means that the lower plotting limit for discharge (`qBottom`) should be set somewhat higher than the minimums for the

dry season of the year and the upper plotting limit for discharge (`qTop`) should be set somewhat lower than the maximums for the wet season of the year.

The choice of time range for the plot is significant. Covering the entire period of record being used in the analysis is valuable from the standpoint of understanding the overall evolution of the system. The negative consequence is that because of the seasonality which is typical of these surfaces, the vertical stripe effect becomes very pronounced and changes, particularly for certain parts of the year, become hard to observe visually. One approach is to first produce a graphic that covers the entire period, and after determining what kinds of changes are of interest, produce another version of the plot which sets the starting and ending dates to cover fewer years (the first two arguments of the function are `yearStart` and `yearEnd`). One can produce a series of such graphics, each one covering a period such as two or three years, forming a progression of plots that could start 5 or 10 years apart in time.

Table 10. Arguments to the `plotContours` function.

Argument	Definition	Default
`yearStart`	Starting date for the contour plot, in decimal years. Should be an integer value.	No default is established, user must set this value.
`yearEnd`	Ending date for the contour plot, in decimal years. Should be an integer value.	No default is established, user must set this value.
`qBottom`	The discharge value that forms the bottom of the plot, expressed in the units specified by `qUnits`. Because of the built-in log scaling these should be values such as 1, 2, 5, 10, 20 50 etc. The function `flowDuration` can be very helpful in specifying an appropriate value for `qBottom`. A good rule of thumb is to set it slightly below the 5% level on the flow duration curve.	No default is established, user must set this value.
`qTop`	Discharge value that defines the top of the plot, expressed in the units specified by `qUnits`. Same issues as discussed above for `qBottom`. A good choice of values is slightly above the 95% level on the flow duration curve.	No default value is defined. User must select.
`whatSurface`	For `whatSurface` = 3 the plotted surface is the expected value of concentration (`ConcHat`). For `whatSurface` = 1 the plotted surface is the values of `yHat` (the expected value of log(concentration). For	`whatSurface` = 3. Plot is the `ConcHat` surface.

	whatSurface = 2 the plotted surface is the SE surface (the standard error of log concentration).	
qUnit	Determines the units to be used for discharge. See printqUnitCheatSheet() for listing of discharge unit codes.	qUnit = 2. Discharge is in m^3/s.
contourLevels	This is a vector of contour level values, typically starting at zero and progressing in equal intervals to some maximum value. However, it need not go to zero and does not have to be equal interval. See text below on how to specify the contourLevels argument.	contourLevels = NA. The contour levels are set by an automatic process. In most cases this is a poor choice (the maximum is set too high), but it can be a good starting point.
span	This argument specifies the smoothness of the flow duration curves plotted on the graph. It is the half window width for computing seasonal flow duration levels.	span = 60. This is generally a good choice and there is typically no need to adjust it.
pval	This is the probability value for the flow frequency information shown on the plot. It specifies the probability of the lower curve (e.g. pval = 0.05 specifies that the lower curve is the 5% level on the seasonal flow duration curve). The upper curve is set at 1 – pval, (e.g. for pval = 0.05, the upper curve would be the 95% level).	pval = 0.05. This is generally a good choice.
vert1	Location of a vertical black line on the graph at a particular time specified by vert1 (defined in decimal years). It is used to illustrate the idea of a "vertical slice" through the contour plot, which might be shown in a subsequent use of plotConcQSmooth.	vert1 = NA. The result is that no vertical line is plotted.
vert2	Location of a second vertical black line on the graph.	vert2 = NA. The result is that no vertical line is plotted.
horiz	Location of a horizontal black line on the graph. It is expressed in the discharge units used in the plot. It can be used to illustrate the idea of a "horizontal slice" through the contour plot, which might be shown in a subsequent use of plotConcTimeSmooth.	horiz = NA. The result is that no horizontal line is plotted.
flowDuration	This is a logical variable. If TRUE the flow duration lines are plotted on the graph. If FALSE they are not plotted.	flowDuration = TRUE.
color.palette	This defines the color palette to be used for the contour levels in the plot, see appendix B for more information	color.palette=colorRampPalette(c("white","gray","blue","red"))

Setting the contourLevels variable is best done using the R function seq. The seq function has three arguments: the first is the starting value in the sequence, the second is the maximum value for the sequence, and the third is the interval between the values in the sequence. Thus, if the desired contours

were at 0, 5, 10, 15, 20, 25, and 30 mg/L, this would be indicated in by `contourLevels = seq(0, 30, 5)`. The plot shown in Figure 36 shows the resulting plot for the Vermilion River nitrate data discussed in the previous section. The command used to produce it is:

```
plotContours(yearStart=1989,yearEnd=1998,qBottom=0.2,qTop=100,contourLevels=seq(0,18,2))  or equivalently plotContours(1989,1998,0.2,100,contourLevels=seq(0,18,2))
```

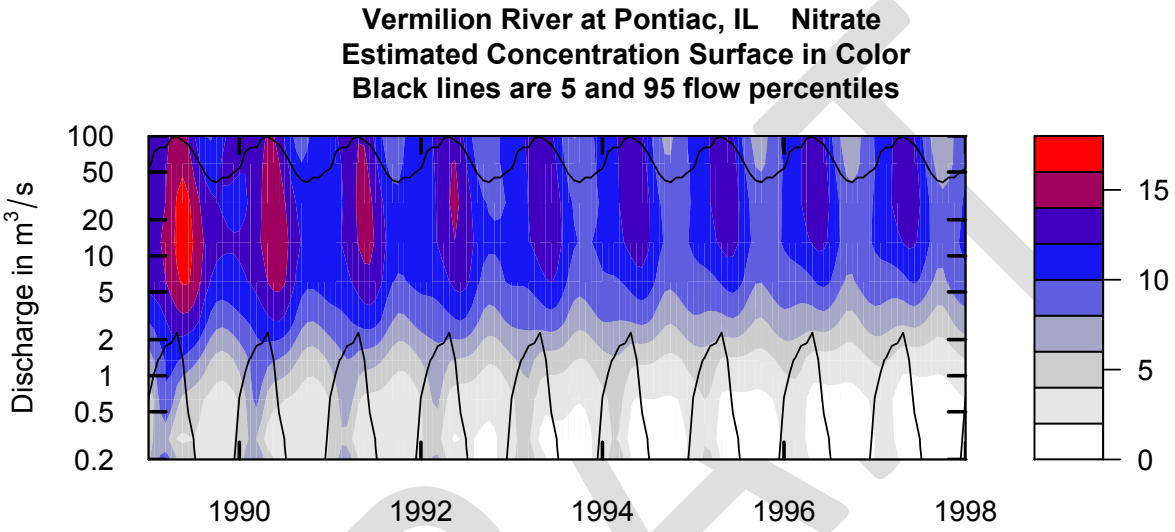


Figure 36. Contour plot for nitrate, Vermillion River at Pontiac, IL. Year designations on the horizontal axis indicate the start of the calendar year.

Setting the best contour intervals is best done by a process of trial and error. The user can start with the default (where `contourLevels = NA`) but the total concentration range used to establish the colors for the contour intervals will probably be too large and will result in very poor differentiation of estimated concentrations at discharges and times of year that are of primary interest. The reason that the default levels go too high is that they are set by the maximum estimated concentrations in the entire Q versus `decYear` domain for the model, which includes some very extreme and very low probability combinations of discharge and season. Assuming an appropriate selection of `qBottom` and `qTop`, the

maximum concentration estimates on the contour plot will often be much lower than the upper value of estimated concentration on the scale bar. By observing the highest estimates plotted when `contourLevels=NA`, the analyst can select a lower maximum value for the scale bar and select a smaller interval between contour levels than those automatically set by default. If the maximum value is not sufficiently high to cover the full range of values, the area that is in excess of the maximum will also be shown in white and the maximum level should be raised to slightly exceed the maximum. The minimum value for the `contourLevels` can be greater than zero, although in many cases zero may be a good choice for the minimum.

Contour plots of the standard error of the WRTDS model (using the argument `whatSurface = 2`) can be useful for purposes of displaying one of the important reasons for using WRTDS versus more standard regression models. That reason is that WRTDS explicitly models the variations in SE. For example, Figure 32 shows a great deal of heteroscedasticity of the residuals in the model whose concentration contours are depicted in Figure 36. Figure 37 shows a two-year example of the WRTDS estimate of the standard error of the model. The command to produce this figure is:

```
plotContours(yearStart=1994,yearend=1996,qBottom=0.2,qTop=100,whatSurface=2,c
ontourLevels=seq(0.2,0.8,0.1))
```

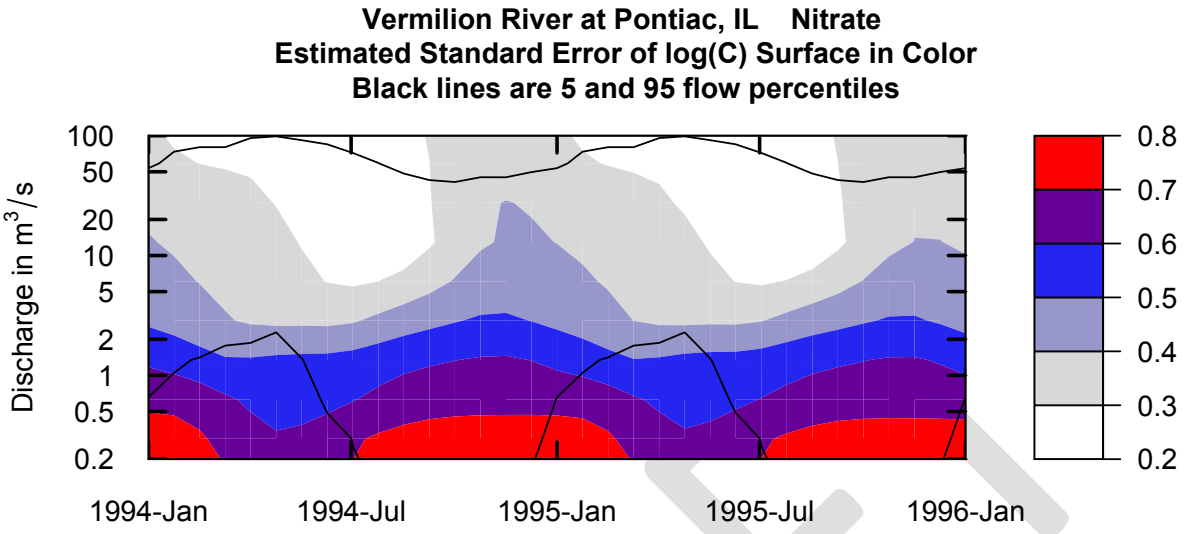


Figure 37. Contour plot of the estimated standard error of log(concentration) using the WRTDS model.

As expected based on the nature of the heteroscedasticity seen in this data set, the *SE* becomes substantially smaller as discharges increase above about 2 m^3/s and the months of late summer and fall have the highest *SE* and the months of spring have the lowest *SE* values. The importance of these variations is related to the computation of the bias correction factor (BCF) for the WRTDS model. As discussed above, the BCF is $\exp(SE^2/2)$. In a standard regression formulation such as the LOADEST models (Runkel and others, 2004), which assumes homoscedastic residuals, the BCF is nearly constant across the range of values of the explanatory variables (see Cohn and others, (1992) for an explanation of the BCF for regression with homoscedastic residuals) . In the case shown here, the BCF for the WRTDS model would vary from 1.331 at very low discharges to 1.020 at very high discharges. A standard regression formulation would have BCF values that range only from 1.208 (at high discharges) to 1.218 (at low discharges). Recalling that the value of `ConcHat` is determined by multiplying

exp(`yHat`) by the BCF these differences in BCF values can be quite significant in determining the estimates of concentration. From a flux estimation perspective, these disparities in BCF values can be of great importance. In this example, at high discharges, which carry most of the flux, the WRTDS BCF is much smaller than the BCF for standard regressions. The result is that standard regressions will seriously over-correct for bias, resulting in a large over-estimate of flux. Conversely, at low discharge the WRTDS BCF is much smaller than the BCF for standard regressions and the result is that the standard regression approach will under-correct at low discharges, but because these low discharges are relatively unimportant to total annual flux. The consequence is that standard regression approaches will over-estimate flux because of their failure to consider heteroscedastic residuals. This issue is discussed in detail in (Hirsch, In Press).

Introducing an example case: Maumee River, Ohio, Dissolved Reactive Phosphorus

The example that will be used to further illustrate the use of `plotContours` and introduce the functions `plotDiffContours`, `plotConcQSmooth` and `plotConcTimeSmooth` is that of Dissolved Reactive Phosphorus (DRP) in the Maumee River at Waterville, Ohio. The data set used here is a subset of the very large data set of 38 years duration collected by the Heidelberg University National Center for Water Quality Research (*http://www.heidelberg.edu/academiclife/distinctive/ncwqr* accessed November, 2013). The full data set consists of 16,930 individual samples collected over the years 1974-1977 and 1980-2012, but what is used here is a randomly selected subset of 1000 of these (to make this more comparable to the types of data sets more commonly encountered, in this case about 27 samples per year). The data set is an interesting case because of the very substantial changes that have taken place over this long period of record and the fact that it illustrates a particularly interesting evolution of water quality issues (Baker and Richards, 2002; Richards and Baker, 2002). Starting in the 1970s DRP was very high and was particularly dominated by point sources, although some DRP came from non-

point sources. The inputs from the Maumee and other major rivers were contributing DRP and other forms of phosphorus that were shown to be a major driver of the severe eutrophication of the western part of Lake Erie. Over a period of several years, substantial investments were made in treating these point sources and as a consequence DRP fluxes from the Maumee River into Lake Erie declined. Along with similar efforts at reducing point sources on other Lake Erie tributaries and the point sources that discharged directly to the Lake, conditions in Lake Erie improved. However, in recent years, non-point sources of DRP have increased due to agricultural practices. These practices include broadcast application of fertilizer onto the surface, application in the fall rather than the spring, allowing both applied fertilizer and crop residue to remain very close to the land surface rather than being incorporated deeper into the soil profile, increased tile drainage, and soil compaction due to heavy equipment. The net effect of these practices is creation of a surface layer of soil with excess phosphorus, which is readily mobilized in the dissolved phase during times of high surface or subsurface flow. As a consequence, conditions in Lake Erie have deteriorated and in the summertime the lake is now severely impaired by algal blooms (especially blue-green algae, some of which are toxic) and hypoxic conditions. The following graphics illustrate the particular tools in WRTDS that can help to elucidate the nature of the long-term changes in DRP flux in the Maumee River.

Because the Maumee River record is quite long, and also contains a substantial break in the monitoring (little or no data in 1978, 1979 and 1980) a useful approach to visualizing the change is to use `plotContours` to consider the relationship of concentration to discharge and time of year for three different periods in the record. The first is 1977-1978, the second is 1988-1989, and the third is 2010-2011. The command to create the first of these is: To create the basic contour plot of this record, the command used is:

```
plotContours(yearStart=1975, yearEnd=1977, qBottom = 20,qTop = 500,
contourLevels = seq(0,0.28,0.04))
```

For purposes of comparison, this plot was combined with the other two time periods to form Figure 38. The contents of the other two contour plots would be obtained by changing the first two arguments (yearStart and yearEnd) to 1988 and 1990 in the second one and 2010 and 2012 in the third one.

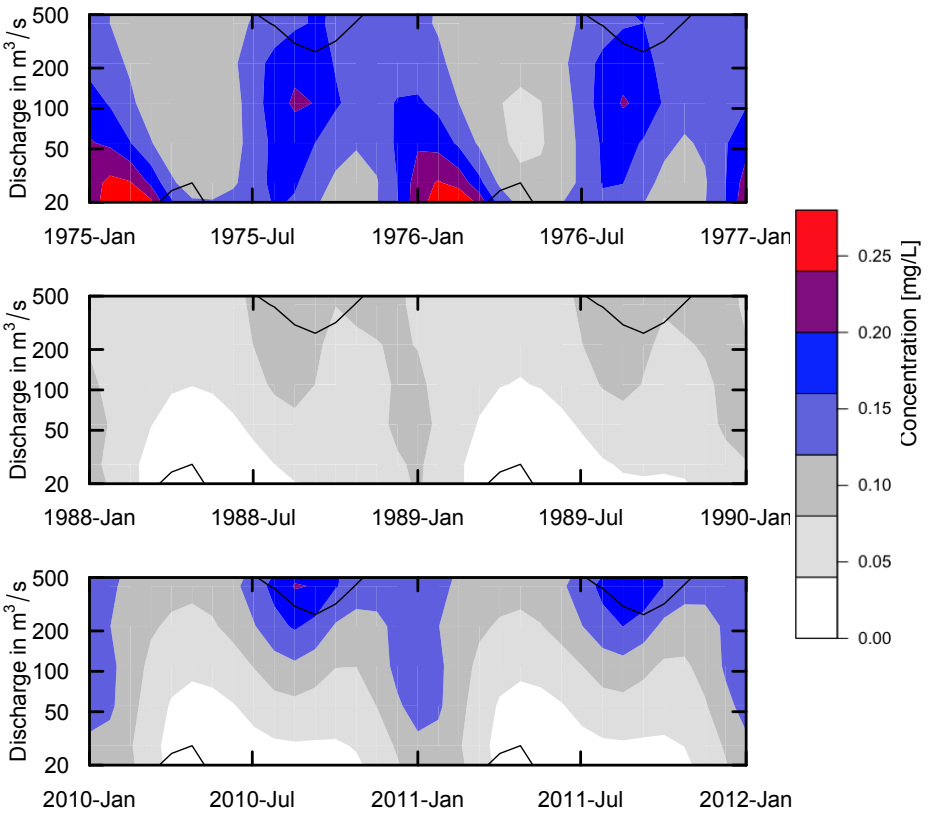


Figure 38. Contour plot of Dissolved Reactive Phosphorus, Maumee River at Waterville, OH, for three, two-year time periods.

The top panel, from the mid-1970s, shows the highest concentrations taking place in the winter months at all flows, but most pronounced at the lowest discharge. This pattern of decreasing concentration with

increasing discharge suggests the importance of point source inputs. Concentrations are also relatively high, almost without regard to discharge during the late summer and early fall, a time when plant uptake of phosphorus from the soil is declining and the harvest of crops and leaf fall creates a large reservoir of available phosphorus on the landscape. Looking next to the late 1980s the situation is quite different. Overall, the concentrations are much lower, there is little indication of major point source inputs, and the highest concentrations of P are during the months of July through January. Finally, the most recent period is similar in nature to the late 1980s but the concentrations at higher discharges are higher than they were in the mid-1980's at all times of the year.

Another way to view the changes that have taken place over some period of time is to use the function `plotDiffContours`. This function computes and plots the difference between the contoured surfaces for any selected pair of years in the record. The arguments to this function are largely the same as those in `plotContours`. Instead of the arguments `yearStart` and `yearEnd`, this function uses `year0` and `year1 to .` The only other difference is that there is no `contourLevels` argument, but in its place is an argument called `maxDiff`. This argument controls the range of contour intervals used in the graphic. The red colors depict the increases over the selected period, and the maximum increase they will depict is equal to `maxDiff`. The blue colors depict the decreases over the selected period and they range from zero to –`maxDiff`. Any region of the contour plot that has a difference that is greater than `maxDiff` in absolute value will be shown in white. If there is an area of white, the analyst should increase `maxDiff` enough so that the graphic contains no white area. The following example, shown in Figure 39, explores the changes from 1988 to 2011. The command used is:

```
plotDiffContours(year0 = 1988, year1 = 2011, qBottom = 20, qTop = 500,
maxDiff=0.12)
```

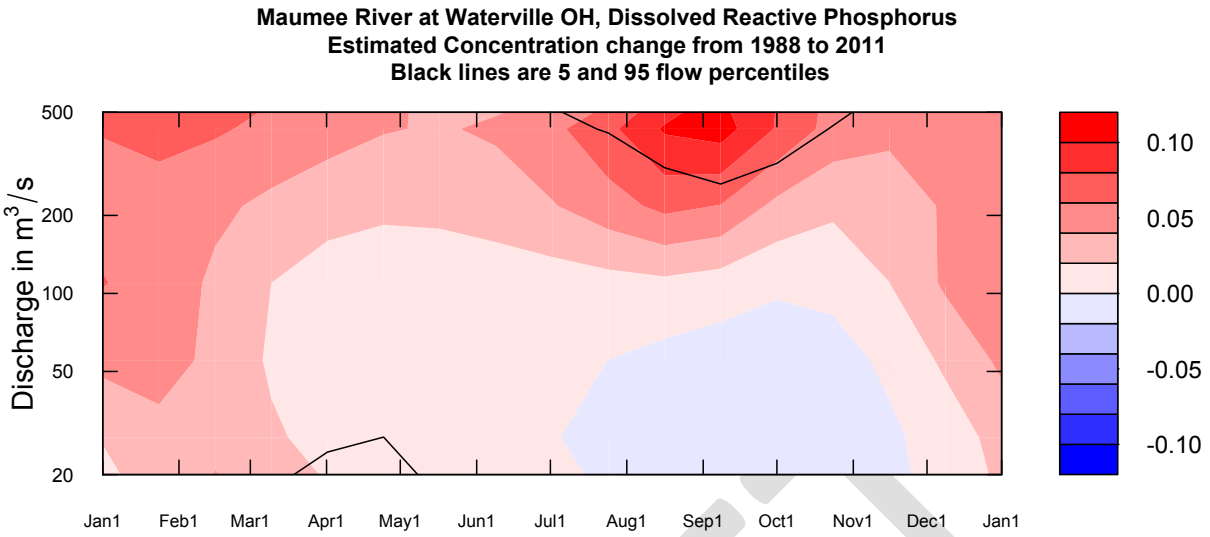


Figure 39. Difference contours for Dissolved Reactive Phosphorus, Maumee River at Waterville, OH, comparing 1988 to 2011.

This figure shows that average concentrations have increased at all discharges during the late fall and through the winter, which is after the fall fertilizer application period and before crop uptake of phosphorus has begun for the growing season. The increases tend to be larger at the higher discharges than at lower discharges. They appear to be largest in the late summer and early fall at the highest discharges. However, it should be noted that these conditions that give rise to the largest increases shown on the figure are highly unusual. They lie above the 95th percentile of the flow duration curve for that part of the year, so these estimates are likely based on relatively few observations in this range, and have very limited influence on average annual concentrations or flux, because they represent conditions that happen with low frequency. The other thing to note from this figure is that there has been very little change in concentration at moderate to low discharges from about April through November and even a small decrease at low discharges in the late summer and fall.

An alternative way to view these surfaces is to plot "slices" through them. The function `plotConcQSmooth`, produces vertical "slices" through the contour plot. It plots the WRTDS estimate of concentration as a function of discharge. It can do so for as many as three different points in time. The arguments to `plotConcQSmooth` are listed and described in Table 11

Table 11. Arguments for the function `plotConcQSmooth`.

Argument	Definition	Default
`date1`	A date, in the form "yyyy-mm-dd" (quotes must be used), specifying a date around which the concentration estimate is to be made using the WRTDS model.	No default is established, user must set this value.
`date2`	A second date, in the form "yyyy-mm-dd", to be used for the second curve on the figure. If no second curve is wanted, then `date2=NA`.	No default is established, user must set this value.
`date3`	A third date, in the form "yyyy-mm-dd", to be used for the third curve on the figure. If no third curve is wanted, then `date3=NA`.	No default is established, user must set this value.
`qLow`	Lowest discharge to be used on figure, expressed in the units specified by `qUnits`. See text below for a discussion of selecting appropriate `qLow` and `qHigh` values.	No default is established, user must set this value
`qHigh`	Highest discharge to be used on figure, expressed in the units specified by `qUnits`. See text below for a discussion of selecting appropriate `qLow` and `qHigh` values.	No default is established, user must set this value.
`qUnit`	Determines the units to be used for discharge. See `printqUnitCheatSheet()` for listing of discharge unit codes.	`qUnit` = 2. Discharge is in m^3/s.
`legendLeft`	The location of the left edge of the legend, expressed in the discharge units used in figure.	`legendLeft` = 0 (this allows the function to set `legendLeft` automatically).
`legendTop`	The location of the top edge of the legend, expressed in concentration units (mg/L).	`legendTop` = 0 (this allows the function to set `legendTop` automatically).
`printLegend`	A logical variable, if TRUE legend is included, if FALSE, legend is not included	`printLegend = TRUE`
`concMax`	Upper bound on the vertical axis for plot. This can be useful when multiple plots are being compared.	`concMax = NA`, which results in the program selecting the upper bound based on the curves being shown.
`concMin`	Lower bound on the vertical axis for the plot. This will be ignored if the vertical scale is arithmetic (`logScale = FALSE`) in which case the lower bound is always 0 mg/L. This can be useful when	`concMin = NA`, which results in the program selecting the lower bound based on the curves being shown (if `logScale = TRUE`), and results in a

	multiple plots are being compared.	lower bound of 0 if `logScale = FALSE`.
`bw`	A logical variable. If `bw = FALSE`, curves are plotted in color. If `bw = TRUE`, curves are plotted in black and white.	`bw = FALSE`
`printTitle`	A logical variable. If `printTitle = TRUE`, title is printed. If `printTitle = FALSE`, title is not printed.	`printTitle = TRUE`
`printValues`	A logical variable. If `printValues = TRUE`, in addition to plotting the graphic, the function prints the values plotted to the console and can create a data frame with these values (see discussion below)	`printValues = FALSE`
`windowY`	Half-window width for time, in years, for the WRTDS smoothing method. (see notes on selection of smoothing parameters below)	`windowY = 10`
`windowQ`	Half-window width for discharge, in natural log units, for the WRTDS smoothing method. (see notes on selection of smoothing parameters below)	`windowQ = 2`
`windowS`	Half-window width for seasons, in years, for the WRTDS smoothing method. (see notes on selection of smoothing parameters below)	`windowS = 0.5`
`minNumObs`	Minimum number of observations required to run a specific weighted regression. (see notes on selection of smoothing parameters below)	`minNumObs = 100`
`minNumUncen`	Minimum number of uncensored observations required to run a specific weighted regression. (see notes on selection of smoothing parameters below)	`minNumUncen = 50`
`logScale`	Logical variable. If `logScale = TRUE` vertical scale is a log scale. If `logScale = FALSE`, vertical scale is arithmetic and starts at 0 mg/L.	`logScale = FALSE`

The selection of values of `qLow` and `qHigh` is facilitated by using the `flowDuration` function. In general, it is best to have the graph cover a range of discharge values that runs from about the 10 percent to 90 percent levels on the flow duration curve that is specific to the time of year that will be portrayed in the graph. For example, if the curves are all set up for August 1 of three different years then the appropriate command to use to identify the `qLow` and `qHigh` would be `flowDuration(centerDate="08-01",span=60)`. This command calls for a flow duration curve specific to dates that are plus or minus 60 days from August 1 of each year of the record, and these will be reported in units of m^3/s (the default for `qUnit` in this function is 2). If other units are going to be used in the `plotConcQSmooth` function, then those units should be specified in the call to

flowDuration using the qUnit argument. If the three dates being used in plotConcQSmooth are for different times of the year, then the choice of qLow and qHigh should be based on the full year flow duration curve, so the command should be flowDuration() (with the qUnit value specified if it is other than m^3/s). In this situation it may be better to use a discharge between the 10 percent and 25 percent levels for qLow and between the 75 percent and 90 percent levels for qHigh.

One example of the use of this function would be to produce a set of three curves depicting the concentration versus discharge relationship in three different years, but all at the same time of year (so the variability due to season is eliminated). The command:

```
plotConcQSmooth(date1="1975-08-01",date2="1988-08-01",date3="2010-08-
01",qLow=10,qHigh=300,
logScale=TRUE,legendLeft=100,legendTop=0.06,printTitle=FALSE)
```

produced the plot is shown in Figure 40. In this case the three dates were chosen to be at August 1 of the first year shown in each of the contour plots in Figure 38. The range of discharge selected for the plot runs from 10 m^3/s to 300 m^3/s. This is approximately the 10 percent to 90 percent range on the flow duration curve for conditions centered on August 1 with a span of 60 days. Setting the range of discharge values for plotConcQSmooth too wide creates the risk that the two ends of each curve will not be particularly meaningful, because they are too heavily influenced by just a few of the highest or lowest discharge sample values. The legendLeft and legendTop values were set after an initial plot was generated without specifying these arguments. The default location had the legend superimposed over two of the curves, so these values were set to assure that the legend would be located in a portion of the figure without any curves. The concentration values are plotted on a log scale (logScale=TRUE).

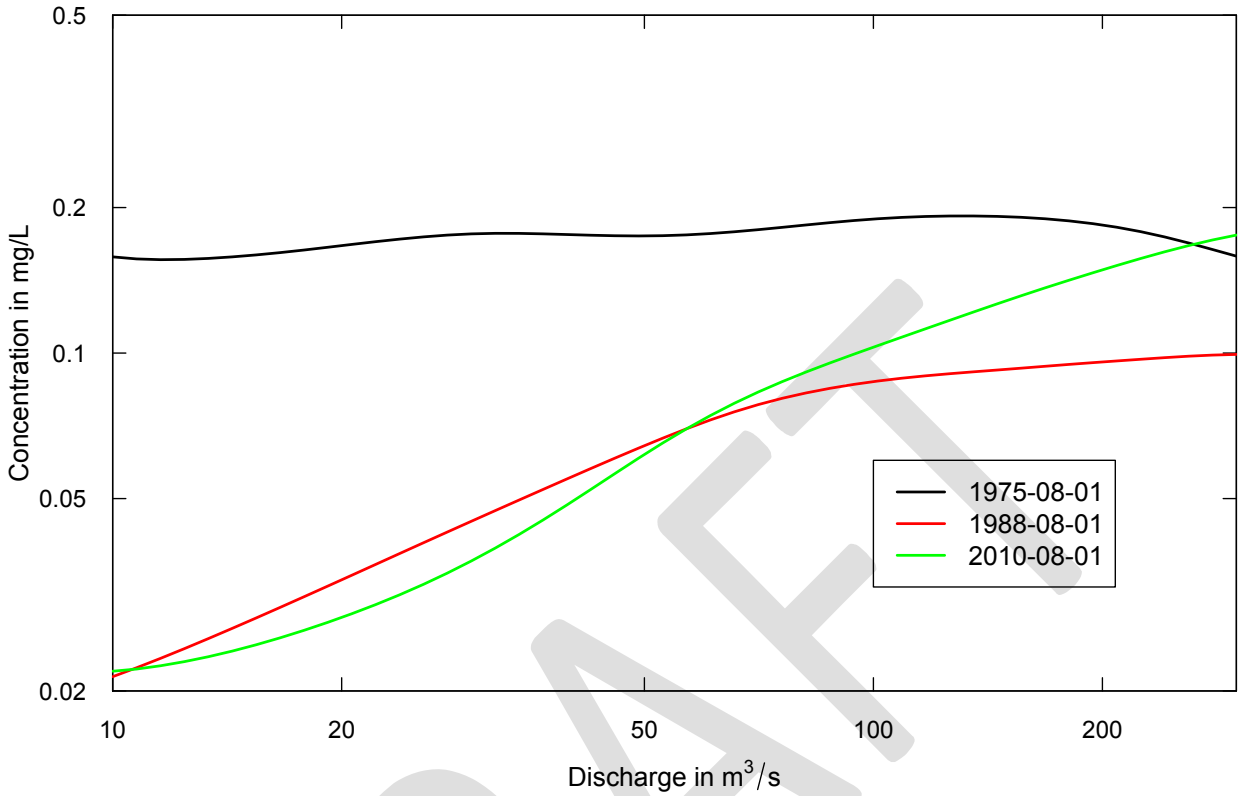


Figure 40. Concentration versus discharge relationship centered on August 1 for three different years, for dissolved reactive phosphorus, Maumee River at Waterville, Ohio.

This graphic describes a very substantial change in the behavior of this watershed over time. The findings mentioned below in the next paragraph were quantified by running another version of the same command:

```
augResults<-plotConcQSmooth("1975-08-01","1988-08-01","2010-08-
01",10,300,printValues=TRUE,logScale=TRUE,legendLeft=100,legendTop=0.06,printTitle=
FALSE)
```

What this command does is that it saves an object, named `augResults` (so named to be suggestive of august results), which is a table of the discharge and concentration values that make up the three curves

(they are a set of 48 discharge values, equally spaced on the log discharge scale between 10 and 300 m^3/s). Then simply typing the command `augResults` prints out this table so that comparisons can easily be made.

What is seen here is that in the early part of the record around 1975, estimated concentrations were relatively constant over the range of discharges, the highest value is only about 23 percent higher than the lowest value. The shape of the curve suggests that dissolved reactive phosphorus (DRP) is derived from a mixture of a constant point source and a non-point source that is highly related to discharge. Thirteen years later, around 1988, the picture is radically different. The highest values of concentration take place at the highest discharges, and these concentrations are about 550 percent larger than the concentrations seen at the lowest discharge. It indicates a decrease in concentrations of about 87 percent at discharges around 10 m^3/s and a decrease of only about 38 percent at the highest discharges. This suggests a very substantial decrease in the point source loading of DRP and a modest reduction in the non-point source loading. Then, moving from 1988 to 2010, the figure suggests that for low and moderate discharges there is very little change in the system over these 22 years, but at discharges above about 100 m^3/s the more recent period had substantially higher concentrations. For example at a discharge of 300 m^3/s the increase is about 76 percent over this period. This indicates that the point source controls seem to continue to be stable and effective, but the non-point sources that drive the DRP concentrations at higher discharges are continuing to increase. So, even though low flow concentrations declined over time and have stayed low, at high flow they appear to have increased a good deal in the later years of this record.

Having made these observations, an obvious next question is: Does the general pattern change if a different time of year is considered. For example, in the following command, the dates are shifted from August 1 to May 1. The command that produced Figure 41. is:

```
mayResults<-plotConcQSmooth("1975-05-01","1988-05-01","2010-05-01", 40, 700,
legendLeft=200,legendTop=0.04,printValues=TRUE,logScale=TRUE,printTitle=FALSE).
```

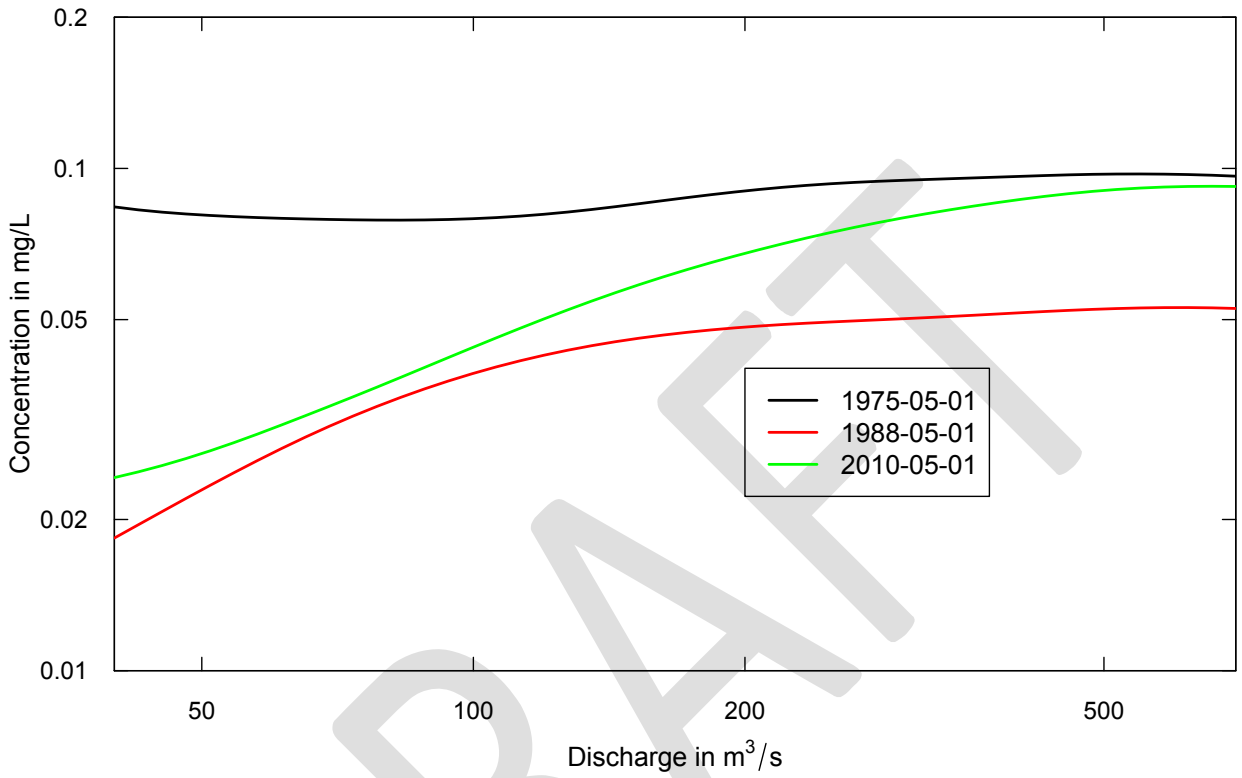


Figure 41. Concentration versus discharge relationship centered on May 1 for three different years, for dissolved reactive phosphorus, Maumee River at Waterville, Ohio.

There are differences in details, between this May plot and the August plot in Figure 40, but the overall message is the same, the concentration versus discharge curve has gone from one that is relatively flat over the relevant range of discharges back in 1975, then it evolves by 1988 to one where the concentrations at low discharges decreased by about 80 percent and concentrations at high discharges also decreased but only by about 50%. However, over time, the concentrations at high discharges have risen such that by 2010 they roughly equal to the high values from back in 1975. The

patterns seen in these two figures provide a very strong case for using WRTDS as a way of describing the evolution of this system, as compared to using LOADEST. LOADEST requires that the shape of the log concentration to log discharge relationship, for any given time of year, must remain the same over the entire period of record. What these figures indicate is that this relationship can dramatically change shape over a period of multiple decades. Using the `tableChanges` function shows that the trend in concentration over the period 1988 through 2010 averaged +1.7 percent per year but the trend in flux for the same period averaged +3.5 percent per year. This is an excellent example of why analysis of concentration trends is not necessarily meaningful for describing trends in flux.

Yet another type of comparison is possible with the `plotConcQSmooth` function, and that is the comparison across different seasons. Figure 42 was produced using the following command:

```
plotConcQSmooth("2010-01-01","2010-05-01","2010-09-
01",30,300,logScale=TRUE,legendLeft=150,legendTop=0.04,printTitle=FALSE)
```

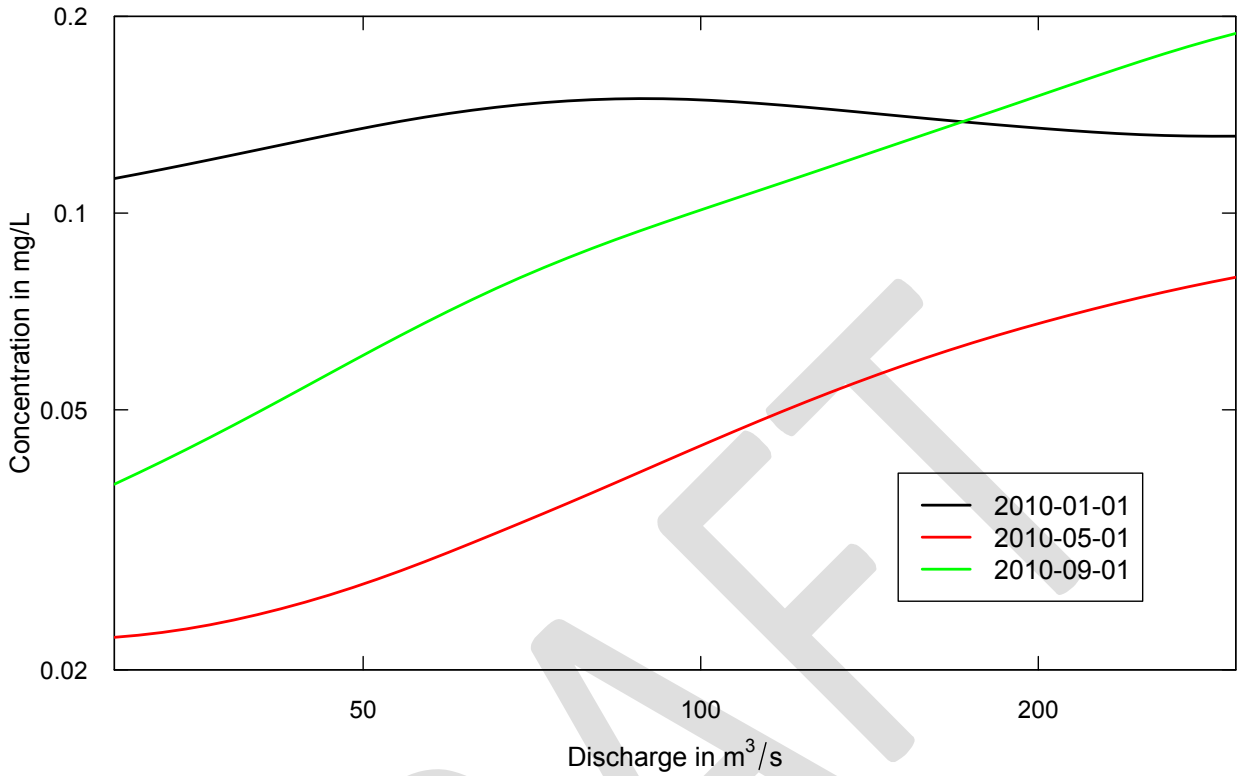


Figure 42. Concentration versus discharge relationship centered on three dates (January 1, May 1, and September 1) of 2010, for dissolved reactive phosphorus, Maumee River at Waterville, Ohio.

Holding the year constant, it simply considers how the concentration versus discharge relationship changes across the seasons, in this case exemplified by the curves for January 1, May 1, and September 1. What Figure 42 shows is that the January curve is nearly horizontal (no change in concentration as a function of discharge) but for May and September the curves rise fairly steeply (increasing by a factor of 4 or 5 over the order of magnitude change in discharge). At lower discharges, the May concentration values are the lowest of the three, reflecting the active plant uptake of phosphorus by plants at this time of year and the fact that the high levels of phosphorus that were available in January have been substantially depleted by May. September values are intermediate and show the likely influence of the

end of the growing season at which time the phosphorus content of the plants becoming available for dissolved transport. Finally, the winter low flows show the effect of minimal plant uptake, the recent fall fertilizer applications and the large amount of dead plant material on the landscape. At higher discharges the concentrations are high both in September and January and somewhat lower in May (associated with plant uptake during the growing season). Making a contrast with the LOADEST approach, LOADEST requires that the log concentration versus log discharge relationship be the same shape and slope across all seasons of the year, and these three curves from the WRTDS model suggest that this may be a very poor model assumption in this particular case.

One additional type of use for the `plotConcQSmooth` function is to allow for experimentation with the setting of the WRTDS smoothing parameters. In particular, there may be an interest in using a smaller window with for discharge (`windowQ`). An alternative version of Figure 42 might use windowQ = 1 (rather than the default value of 2). Figure 43 was created with the command:

```
plotConcQSmooth(date1="2010-01-01",date2="2010-05-01",date3="2010-09-
01",qBottom=30,qTop=300,logScale=TRUE,legendLeft=150,legendTop=0.04,printTitle=FALS
E, windowQ=1).
```

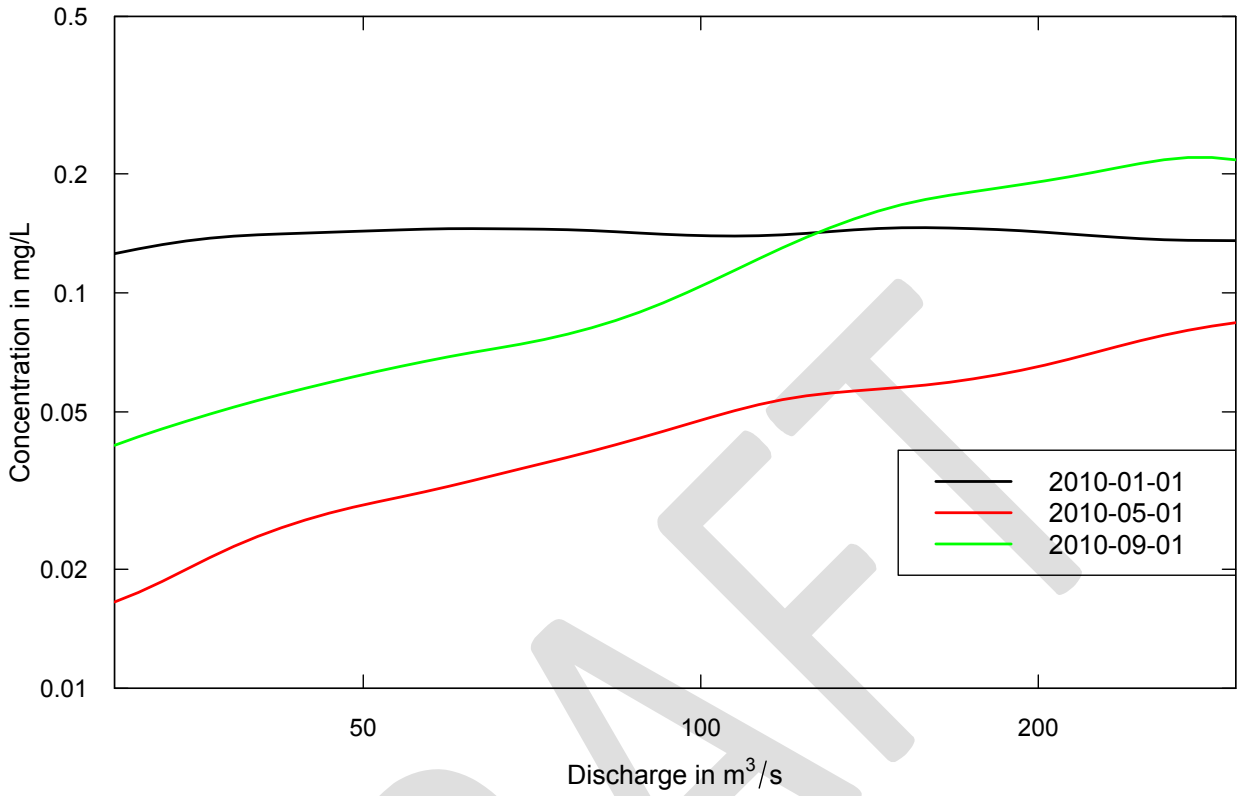


Figure 43 Concentration versus discharge relationship centered on three dates (January 1, May 1, and September 1) of 2010, with the discharge smoothing parmeter (windowQ = 1 rather than windowQ = 2) for dissolved reactive phosphorus, Maumee River at Waterville, Ohio.

Figure 43 is not dramatically different from Figure 42, but subjectively the original (with `windowQ = 2`) seems more plausible. The slightly wavy curves shown in Figure 43 seem to invite an over-detailed interpretation of the data. The selection of "optimal" window widths remains a research challenge for the WRTDS method, but extensive experimentation has indicated that the default values provide results that are about as accurate as the method can obtain. As described in Hirsch and others (2010) and Sprague and others (2011), there may be situations on very large rivers (e.g. the Mississippi

or Missouri Rivers) where `windowQ = 1` or `1.5` may perform better than `windowQ = 2`, but this does not appear to be the case for this example.

There are situations, particularly when the data set is small (say 100 or 200 observations) or the curves are being extended to a range where there are very few observations, that the curves produced take on a "sawtooth" appearance, rather than the smooth behavior observed in these examples. The following command produces such an example:

```
plotConcQSmooth("2010-04-01","2010-08-01","2010-12-01", 1, 300,
legendLeft=10, legendTop=0.19)
```

The result is depicted in Figure 44.

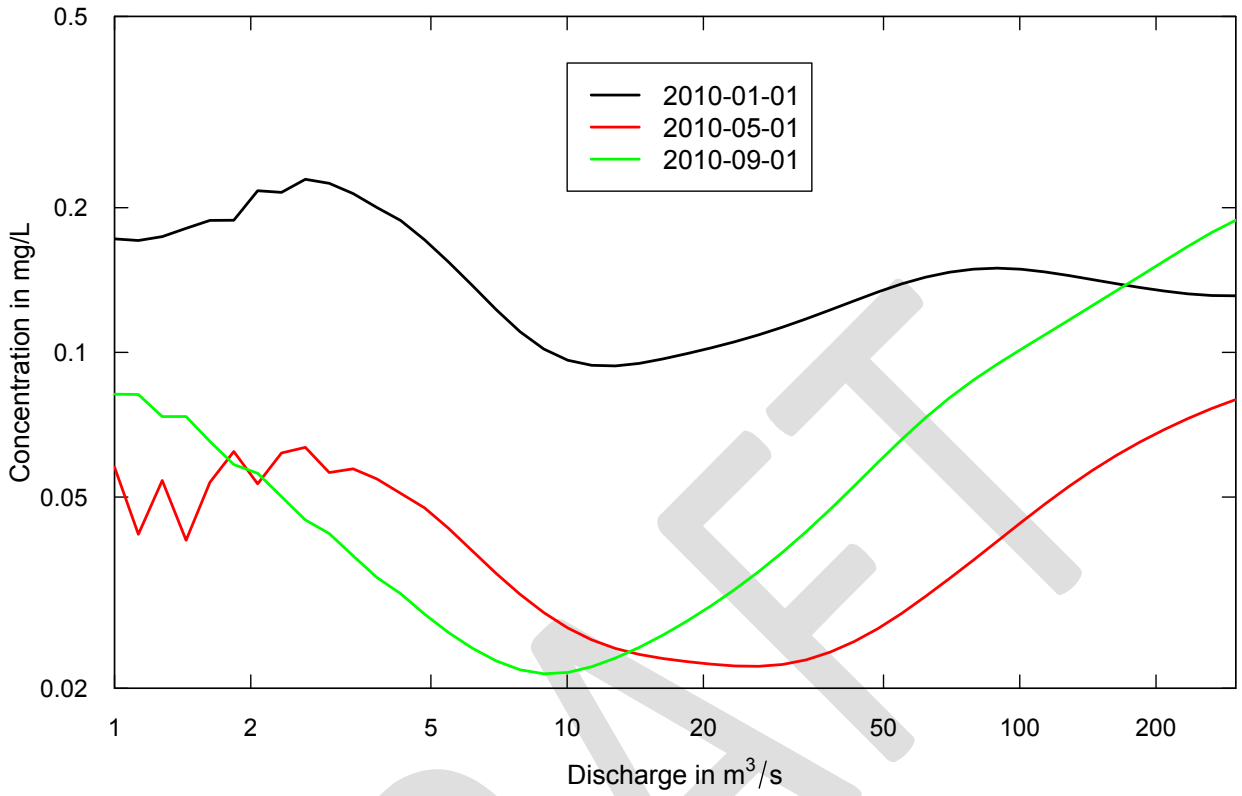


Figure 44. Concentration versus discharge relationship centered on three dates (April 1, August 1, and December 1) of 2010, for dissolved reactive phosphorus, Maumee River at Waterville, Ohio, but shown with a discharge scale extended to excessively low values.

The explanation of the sawtooth pattern at the lowest discharge values is that the estimates represented by these curves particularly below discharge values around 8 m^3/s are at such extreme edges of the full sample data set that the WRTDS algorithm has to widen the windows (one or more times) in order to obtain the required 100 observations with non-zero weights. This incremental widening creates a series of oscillations in the curves that are just an artifact of the widening algorithm. Typically, when these kinds of oscillations happen, it is because the range of discharge values considered goes too far towards the extremes of the data set. For example in this case, the lowest observed discharge in the

sample data set is 1.56 m^3/s, so the curves are extending into a range where there are very few observations. Resetting the `qLow` argument to 30 resolves this problem for this data set.

In any given application of the WRTDS model there will be portions of the model domain where the combination of discharge and time of year are such that the available data that are close to those values are very limited and the kind of oscillatory behavior shown here does influence the values that are stored in the `surfaces` matrix. This has two consequences. One is that plotted versions of the surfaces can be rather unreliable at the most extreme low or high discharges. It is for this reason that applications of `plotContours` and `plotDiffContours` should not encompass the full extent of the domain over which they were calculated, but should be compressed to the more common values (say between the 5 percent and 95 percent values on the flow duration curve, and if possible, avoid the first and last years of the data set). The other consequence is that they will influence the computation of estimated concentrations and fluxes. While these can have a moderately large influence on individual daily estimates, when they are aggregated into monthly or annual mean values of concentration or flux, these oscillations should balance out and have very little influence on these aggregated results. Sensitivity tests have shown that annual results are rather insensitive to reasonable modifications of the smoothing parameters even though they can cause a noticeable change in these `plotConcQSmooth` graphs.

When data sets are rather small (for example less than 100 observations) the two arguments `minNumObs` and `minNumUncen` may need to be reduced from their default values (100 and 50 respectively). Using them in `plotConcQSmooth` graphs can indicate the degree of sensitivity of results to these changes. One thing to recognize about all of these adjustments of the smoothing parameters in this function is that the results are not derived from the smooth estimated concentration surfaces stored in the object `surfaces`. These `plotConcQSmooth` curves are calculated by performing the weighted

regressions at each of 48 discharge values for each curve plotted and they use whatever smoothing parameters are specified in the command given. Changing these parameters in `plotConcQSmooth` will not result in a change in the surfaces object and hence not result in any changes in the calculated monthly or annual results. If these plots suggest the need to change the smoothing parameters to be used to compute the WRTDS results, the function `modelEstimation` must be re-run with the desired smoothing parameters (the arguments `windowQ, windowY, windowS, minNumObs,` and `minNumUncen`). When `modelEstimation` is re-run with new parameters, these parameter values will all be stored in the `INFO` data frame, and new versions `of Sample, Daily, surfaces`, and `AnnualResults` will all replace the versions that had been computed the last time `modelEstimation` was run.

plotConcTimeSmooth

As its name suggests, this function operates very similarly to `plotConcQSmooth`, but "slices" the contour plot in the horizontal direction. However, if one were to take a slice through the contour plots at a given discharge across the full time range, the resulting curve would show a strong seasonal pattern. In order to focus on the long-term trend pattern this seasonal oscillation is eliminated by the selection of a particular day of the year to be plotted. A way to think about the construction of this graphic is this. If one plotted a horizontal line at a selected discharge value, and then plotted a set of vertical lines, on a given day of the year for every year in the record, the `plotConcTimeSmooth` graph would capture the value of estimated concentration at every intersection of the horizontal and vertical lines. This can be done for as many as three different discharge values in one graph. Caution should always be used in interpreting these curves near the starting and ending dates of the data set. Smoothing algorithms, such as the one used here, will always be less reliable at the extreme ends of the record than they are in the middle. Many of the arguments that are used in `plotConcQSmooth` are used in this function, but for the

sake of completeness here, the information about all of the arguments is presented here as they were in Table 12.

Table 12. Arguments for the function `plotConcTimeSmooth`

Argument	Definition	Default
`q1`	The discharge, in units specified by `qUnit`, which specifies the discharge for the first curve on the figure.	No default is established, user must set this value.
`q2`	The discharge, in units specified by `qUnit`, which specifies the discharge for the second curve on the figure. If a second curve is not to be plotted, then `q2` should be set to NA.	No default is established, user must set this value.
`q3`	The discharge, in units specified by `qUnit`, which specifies the discharge for the third curve on the figure. If a third curve is not to be plotted, then `q3` should be set to NA.	No default is established, user must set this value.
`centerDate`	This argument sets the month and day of the year for which all of the curves are to be computed. The argument must be specified in the form "mm-dd", thus if the curve is to be computed for May 15 of every year, `centerDate = "05-15"` (it must be in quotes).	No default is established, user must set this value
`yearStart`	This is the starting year for the graph. The first plotted value will be on the first `centerDate` after the time specified by `yearStart`.	No default is established, user must set this value.
`yearEnd`	This is the ending year for the graph. The last plotted value will be on the `centerDate` prior to the time specified by `yearEnd`.	No default is established, user must set this value.
`qUnit`	Determines the units to be used for discharge. See `printqUnitCheatSheet()` for a list of discharge unit codes.	`qUnit = 2`. Discharge is in m^3/s.
`legendLeft`	The location of the left edge of the legend, expressed as time in years.	`legendLeft` = 0 (this allows the function to set `legendLeft` automatically).
`legendTop`	The location of the top edge of the legend, expressed in concentration units (mg/L).	`legendTop` = 0 (this allows the function to set `legendTop` automatically).
`printLegend`	A logical variable, if `TRUE` legend is included, if `FALSE`, legend is not included	`printLegend = TRUE`
`concMax`	Upper bound on the vertical axis for plot. This can be useful when multiple plots are being compared.	`concMax = NA`, which results in the program selecting the upper bound based on the curves being shown.
`concMin`	Lower bound on the vertical axis for the plot. This will be ignored if the vertical scale is arithmetic (`logScale = FALSE`) in which case the lower bound is always 0 mg/L. This can be useful when multiple plots are being compared.	`concMin = NA`, which results in the program selecting the lower bound based on the curves being shown (if `logScale = TRUE`), and results in a lower bound of 0 if `logScale = FALSE`.
`bw`	A logical variable. If bw = FALSE, curves are	`bw = FALSE`

	plotted in color. If bw = TRUE, curves are plotted in black and white.	
printTitle	A logical variable. If printTitle = TRUE, title is printed. If printTitle = FALSE, title is not printed.	printTitle = TRUE
printValues	A logical variable. If printValues = TRUE, in addition to plotting the graphic, the function prints the values plotted to the console and creates a data frame with these values (see discussion below)	printValues = FALSE
windowY	Half-window width for time, in years, in the WRTDS smoothing method. (see notes on selection of smoothing parameters below)	windowY = 10
windowQ	Half-window width for discharge, in natural log units, for the WRTDS smoothing method. (see notes on selection of smoothing parameters below)	windowQ = 2
windowS	Half-window width for seasons, in years, for the WRTDS smoothing method. (see notes on selection of smoothing parameters below)	windowS = 0.5
minNumObs	Minimum number of observations required to run a specific weighted regression. (see notes on selection of smoothing parameters below)	minNumObs = 100
minNumUncen	Minimum number of uncensored observations required to run a specific weighted regression. (see notes on selection of smoothing parameters below)	minNumUncen = 50
logScale	Logical variable. If logScale = TRUE vertical scale is a log scale. If logScale = FALSE, vertical scale is arithmetic and starts at 0 mg/L.	logScale = FALSE

Using the following as the command:

```
plotConcTimeSmooth(q1=5, q2=35, q3=250, centerDate="09-01", yearStart=1975,
yearEnd=2010, logScale=TRUE, legendLeft=1975.5, legendTop=0.018, printTitle=FALSE)
```

results in the graphic shown in Figure 45.

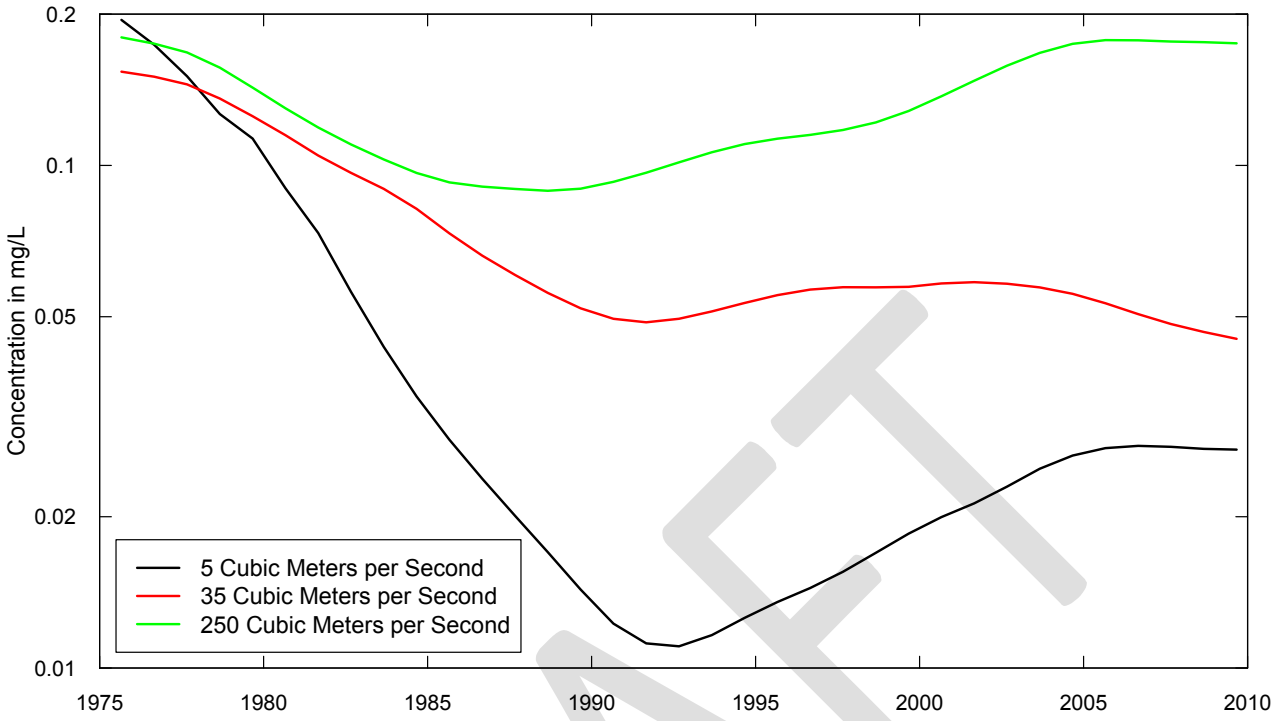


Figure 45. Concentration versus time plots for 3 different discharge values, for dissolved reactive phosphorus, Maumee River at Waterville, Ohio, centered on September 1 of each year

What the plot reveals is that for late summer conditions, concentrations of DRP declined very markedly for low discharge values (5 m^3/s which is near the 5th percentile point on the seasonal flow duration curve) from 1975 to 1992 with a total decline of about 94 percent followed by an increase of about 150 percent from 1992 to 2009. Over the entire time period the decrease is about 86 percent. At a moderate discharge (35 m^3/s which is slightly greater than the median discharge for this time of year) the decline was also substantial (a decrease of 71 percent) with most of that decrease focused in the years leading up to 1992. Since that time, the mean concentration at this time of year and discharge has been relatively steady. However, for high discharge values (250 m^3/s which is the 95^{th} percentile of the

seasonal flow duration curve) the decline from 1975 through 1988 was about 50 percent, but for the entire period, from 1975 to 2009 there has been virtually no change in the mean concentration for this discharge and time of year.

This example is illustrative of just how different the patterns of trend can be across the range of streamflow conditions. The widely-used LOADEST model assumes that trends in log concentration are quadratic in shape (these are certainly not quadratic) and that they assume the same shape regardless of discharge (again, very far from true). The Maumee River is an example where there has been great success in reducing point source contributions but the non-point sources, which are most important at high discharge, have increased over time. It also illustrates just how different trends in concentration can be from trends in flux. In this case, using the function `tableChange`, the increase in flow-normalized concentration from 1987 to 2004 is estimated to be 19 percent, but the increase in flow-normalized flux over this same period is estimated to be 63 percent. This example shows that making inferences about flux change based on estimated changes in concentration is not justified, and that graphics such as `plotConcTimeSmooth` can help elucidate why they may be quite different.

Editing data sets

The R programming language is a very powerful environment for data manipulation. There are many helpful resources available in books and websites. A few simple examples will be given here, but these examples are in no way a comprehensive introduction to R data manipulation.

The structure of many of the EGRET objects as described throughout this report are data frames. To introduce some basic concepts of data frames, let us assume we have a data frame called `DF`. In data frame `DF`, there are three columns: `Date`, `Value`, and `Qualifier`. An individual entry in the data frame can be called in several ways. One is to use a single bracket, with 'row,column' defined inside. For

example `DF[1,2]` outputs the first row, second column. Therefore, if we wanted to simply view the data for that cell, we could type:

```
DF[1,2]
```

If we wanted to adjust the value in that cell, we could assign a new value:

```
DF[1,2] <- 5
```

With this convention, we could also get all rows of the second column:

```
DF[,2]
```

Or, all columns of a particular row (the first row in this example):

```
DF[1,]
```

Another way to view the same data is to use the column name. `DF$Value` would return a vector with all the values of the column 'Value'. To view the same data as above (`DF[1,2]`), we could also use the command:

```
DF$Value[1]
```

If we want to adjust the value to that cell, we could assign a new value:

```
DF$Value[1] <- 6
```

R also lets you put logical statements within the square brackets. So, if you wanted a subset of data that was greater than 10, you could use the command:

```
DF[DF$Value > 10,]
```

If we wanted to replace values less than 10 with 10, and those same rows, change the `Qualifier` to "<", the following commands would work:

```
DF$Value[DF$Value < 10] <- 10
DF$Qualifier[DF$Value < 10] <- "<"
```

With this basic knowledge of R data frame structure, we can work through a few examples that might come up in an EGRET analysis.

Deleting values

If we had some reason to believe that all the samples above 100 were suspect, we could delete those rows from the `Sample` data frame:

```
Sample <- Sample[Sample$ConcAve < 100,]
```

There is also function built into R, `subset`, that would accomplish the same goal:

```
Sample <- subset(Sample,ConcAve < 100)
```

Shortening the Period of Record

In the `Daily` and `Sample` data frames, there is a column called `Date`. This column is in an R date structure, which is to say there is more information there than just the character string. We can compare the dates in the `Date` columns with other dates. The simplest way to create an R date object is to use a string in the format "YYYY-MM-DD", enclosed in `as.Date()`. If we had a `Sample` data frame, and we wanted to remove all samples that were collected before Jan. 1, 1980, we could use the following command:

```
smallSample <- Sample[as.Date("1980-01-01") < Sample$Date,]
```

or:

```
smallSample <- subset(Sample,as.Date("1980-01-01") < Date)
```

Create interval concentrations

Recalling Figure 13, which shows the full set of concentration data for the Choptank River at Greensboro, MD, it was clear from the figure that the rounding convention for reporting the data changed around 1994. For the earlier part of the record, values measured at 1.0 mg/L or greater were rounded to the nearest 0.1 mg/L, lower values or those that came later in the record were reported to a higher degree of precision (generally the nearest 0.01 mg/L). It might be of interest to consider a way of expressing the values from the earlier period that reflects the true degree of precision. This could be

done by considering those rounded values to be interval censored data with the interval covering a range from 0.05 mg/L below the reported value to 0.05 mg/L above the reported value (so a value reported as 1.2 mg/L becomes an interval of 1.15 to 1.25 mg/L). The following steps could accomplish this kind of change.

```
Sample$ConcLow <- ifelse(as.Date(Sample$Date) < "1994-10-01" & Sample$ConcLow
>= 1.0, Sample$ConcLow-0.05, Sample$ConcLow)
```

The `ifelse` function is a way of applying some logical test to a vector of values and in the vector returned it is set to one value if the answer is TRUE and another value is the answer is false. In this case it is being used to reset the values in `Sample$ConcLow`. The test checks two conditions, the first being that the date is before 1994-10-01 and the second is that the existing value of `Sample$ConcLow` is greater than or equal to 1. If these two conditions hold then we want to apply interval censoring and if one or both of the conditions do not hold then we do not want to apply interval censoring. In the TRUE case we set the new value to be 0.05 below the reported value of `Sample$ConcLow`. In the FALSE case we leave the `Sample$ConcLow` value at its existing value.

The next step is to make the same test and adjustment to `Sample$ConcHigh`. The command is very similar:

```
Sample$ConcHigh <- ifelse(as.Date(Sample$Date) < "1994-10-01" &
Sample$ConcHigh >= 1.0, Sample$ConcHigh+0.05, Sample$ConcHigh)
```

Now, having made changes in some of the `Sample$ConcLow` and `Sample$ConcHigh` values the `Sample$ConcAve` and `Sample$Uncen` values need to be re-computed and stored in the revised data frame. The function `fixSampleFrame` will accomplish this. The command, to accomplish this is:

```
Sample <- fixSampleFrame(Sample).
```

These are just a few examples of how R functions can be used to make certain kinds of edits to the data. It is often wise to keep a copy of the data set as it was before any editing was done. This is

easily accomplished in R by making a copy of the specific data frame to keep and not edit at all. For example, if we want to keep a copy of Sample in its original form we could create a new data frame called `keepSample` by giving the command:

```
keepSample <- Sample
```

Then we would proceed to do our editing on the version called `Sample`. If later on, we wished to revert back to using the original data frame version of the data set, this could be accomplished with the command:

```
Sample <- keepSample.
```

Working with multiple versions of data frames

At times the user might want to compare results for the same site and variable of interest, where the comparison might be the use of somewhat different data sets or method of analysis (e.g. different choices of window widths). This can be facilitated by making use of alternative data frames. In reality these could be alternative objects that aren't strictly data frames. For example they might be an array like `surfaces`, but for simplicity here they will be referred to as data frames. The key to this process is to have these alternative data frames structured like one of the standard data frames. For example, we have the `Sample` data frame, and it has a standard set of variable names such as `Sample$Date`, `Sample$Q`, `Sample$ConcLow`, etc. The alternative data frame might be called `shortSample` (named so because we are curious about how our analysis results would behave if we left off the first few years or last few years of data). `shortSample` would have variables within it with names just like Sample: `shortSample$Date`, `shortSample$Q`, `shortSample$ConcLow`, etc.

EGRET functions generally contain input arguments that default to `Sample`, `Daily`, `INFO`, `annualSeries`, etc. In the help files for each function (viewed by typing ?functionName in the R

environment), there is a 'Usage' section that shows all of the function arguments with their defaults. For example, `printSeries` shows in the 'Usage' section:

```
  printSeries(istat, qUnit = 1, runoff = FALSE,
localINFO = INFO, localAnnualSeries = annualSeries)
```

This indicates that the first argument that the function requires is the `istat` variable, the second is `qUnit`, which defaults to `1`, `runoff` which defaults to `FALSE`, `localINFO` defaults to `INFO`, and `localAnnualSeries` defaults to `annualSeries`. If the user only wanted to change the `runoff` argument to `TRUE` with an `istat` number of `2`, the call to the function would be:

```
printSeries(2, runoff = TRUE)
```

The value for `istat` in this case will be `istat=2` because the function requires that the first input is the `istat` value. However, since the rest of the input arguments have preset defaults, it is required to specify which argument is being adjusted (in this case, `runoff`). Therefore, using alternative versions of the `Sample`, `Daily`, and `INFO` data frames usually just require specification of the `localSample`, `localDaily`, or `localINFO` variables (the 'local' naming convention was picked to differentiate what data frames the functions use within the function, in contrast to the names of those data frames in the global environment).

The `modelEstimation` function has an additional behavior concerning default function input arguments. When `localDaily`, `localSample`, or `localINFO` are defined (i.e. not using defaults), the data frame that is assigned is also modified during the execution of the function. For example, 3 columns are added to the `Sample` data frame (`yHat`, `SE`, and `ConcHat`) and 6 columns are added to the Daily data frame when `modelEstimation` is executed. If a data frame named `smallSample` were to be used instead of the default `Sample`, then `smallSample` would have the additional columns upon completion of the `modelEstimation` function. Similarly, if a data frame named smallDaily were to be used instead of the default Daily, then smallDaily would have the additional columns upon completion

of the modelEstimation function. Additionally, `modelEstimation` also creates an array normally called `surfaces`, and a data frame normally called `AnnualResults`. If the user wanted these names to be something else, they could be defined in the `localSurface` and `localAnnualResults` arguments. For example, if there were data frames called `smallSample and smallDaily` being used, and we wanted the `surfaces` and `AnnualResults` returned as `smallSurfaces` and `smallAnnual`, the command for `modelEstimation` would be:

```
modelEstimation(localSample=smallSample, localDaily=smallDaily,
localSurface="smallSurfaces",localAnnualResults="smallAnnual")
```

Note that it may seem odd that the names of some of the objects specified it this command are in quotes and others are not. The ones in quotes are those objects that do not already exist.

Let's look at a real example. In the Choptank River example, we retrieved all of the samples back to 1979-09-01. But, let us say that we are looking at this as a part of a larger study, and the other records in the study didn't start until water year 1985, and we want to consider the idea that we might want to leave out the Choptank data prior to 1985 and see if it substantially influences our results. First, a comment about this question: It is certain that there will be some influence on the later results because the model for 1985 and beyond is influenced by data from before 1985 (because of the windows). The question is, how large is that influence? A second comment is that there is probably no right or wrong answer as to how to proceed with such a study. The case for using the earlier data is that one should always work with the greatest amount of information available. The case against is that if we used the earlier data then this one site would show behaviors around 1985 that are influenced by events (regional climatic events and/or regional changes in land use or cultivation practices) that preceded 1985 but they were excluded from the other data sets, because such data were not available. In any event, we may wish to make this long-record/short-record comparison. Let us assume here that we have already run

the retrievals and fit the model and have created the `Sample, Daily`, and `INFO` data frames and the results in the form of `surfaces` and `AnnualResults`.

Now, to have analyses for the short record we would create modified versions of our data frames as follows:

```
smallStartDate<-"1984-10-01"
smallSample<-Sample[as.Date(Sample$Date) > smallStartDate,]
smallDaily <- Daily[as.Date(Daily$Date) > smallStartDate,]
```

We might also want to check to make sure that the new versions were created correctly by running the following commands (shown here to compare `smallSample` to `Sample`, but the same set of commands should also be run on `smallDaily` and `Daily`).

```
summary(smallSample)
length(smallSample$Date)
summary(Sample)
length(Sample$Date)
```

Now, let's pause and consider what is going on here. We have created a new object for the 1984-10-01 starting date, and using it we have created a new data frames called `smallSample` and `smallDaily` which are structured like `Sample` and `Daily` respectively but have a more limited time range. Then when calling the various function we need to use the arguments `localSample` and `localDaily` if we want that function to use these new data frames. Up to this point in the manual we have always allowed these arguments like `localSample` or `localDaily`, to be equal to their default value (e.g. `localSample = Sample`). Now that we have created these new, alternative, data frames we need to specify them when calling a function and put in these arguments.

The command:

```
modelEstimation(localSample=smallSample, localDaily=smallDaily, localSurface
= "smallSurfaces", localAnnualResults="smallAnnual")
```

will draw upon `smallSample` and `smallDaily` for the data, and will return results in all four of the data frames named in the call (`smallSample, smallDaily, smallSurfaces,` and `smallAnnual`).

Now, if we want to use these new results make a graph of the flux history: we could make the plot as follows.

```
plotFluxHist(1985,2012, localDaily = smallDaily)
```

and compare that to the version that uses the older data

```
plotFluxHist(1985,2012)
```

or equivalently

```
plotFluxHist(1985, 2012, localDaily = Daily)
```

This would have created the two versions of the same graph, based on the different set of results. This same idea applies to any one of the graphical or table outputs. They can be run on each of the several data sets and see what the differences look like.

There is an alternative to this approach and that is to save the results of one analysis (using `saveResults`) and starting all over with a fresh data retrieval and save those results (again, using `saveResults`). The caution here is that there needs to be a way of distinguishing between the two saved workspaces. This can easily be achieved during the use of `getMetaData`. When it calls for abbreviations for the data set, the user can specify something in the station or parameter abbreviation that will make it possible to distinguish between the two different workspaces.

Batch processing in EGRET

When running a large number of analyses the EGRET code can be run in batch mode. The way this is done is to create a text file that contains the sequence of commands that are to be run and this file

can then be run using the `source` function in R. The process of creating the initial workspace (the data frames `Sample`, `Daily`, and `INFO`) are best done interactively, although they can be done in batch. The reasons for doing these steps interactively are 1) these steps typically take very little computer time and 2) the interactive approach is more conducive to identify data problems such as highly unusual data values or record lengths that are different from what may be needed for the analysis being planned. Running the process through the step of `multiPlotDataOverview` gives the analyst several opportunities to spot problems with the data set that need to be explored and corrected.

Let's assume that we have created two workspaces: call them `CHOP.TN.RData` and `SUSQ.TN.RData` (the first being for Choptank River total nitrogen, the second being for Susquehanna River total nitrogen) and these workspaces each have the `Sample`, `Daily`, and `INFO` data frames in them and everything is ready for running model estimation and looking at results. Let's assume that the user has a directory where these workspaces are saved and the object `savePath` has been defined with a command like:

```
savePath<-"/Users/rhirsch/Desktop/examples/"
```

Here is what the file of commands might look like:

```
library(EGRET)

fileName<-paste(savePath,"CHOP.TN.RData",sep="")
load(fileName)
modelEstimation()
tableChange(fluxUnit=5,yearPoints=c(1980,1990,2000,2010)
tableResults(qUnit=1,fluxUnit=5)
saveResults(savePath)

fileName<-paste(savePath,"SUSQ.TN.RData",sep="")
load(fileName)
modelEstimation()
tableChange(fluxUnit=6,yearPoints=c(1980,1990,2000,2010))
tableResults(qUnit=3,fluxUnit=6)
saveResults(savePath)
```

The same effect can also be achieved by using a loop, especially useful if running a large number of EGRET analyses:

```
library(EGRET)
savePath<-"/Users/rhirsch/Desktop/examples/"
filesToOpen <- c("CHOP.TN.RData","SUSQ.TN.RData")
flux <- c(5,6)
q <- c(1,3)

for (i in 1:length(filesToOpen)){
      fileName<-paste(savePath, filesToOpen[i],sep="")
      load(fileName)
      modelEstimation()
      tableChange(fluxUnit=flux[i],yearPoints=c(1980,1990,2000,2010))
      tableResults(qUnit=q[i],fluxUnit=flux[i])
      saveResults(savePath)
}
```

This code will load the workspace, run the WRTDS analysis, provide tabular output (to the console) in the form of changes and listings of the data, and then re-save the workspaces objects such as `Sample` and `Daily` augmented with the results of the analysis. Note that some of the options in the table commands are different because the rivers are of very different sizes so we might want to see flux in tons/year for the Choptank and thousands of tons per year for the Susquehanna. Later on, the workspaces that were saved can be reloaded and a variety of plots can be made. Note that most of the batch commands are just a repetition of steps and only a few differences need to be entered to make up a long file of many analyses. Then, if we name this file "exampleCommands.txt" then all we need to do once we start up R is to give the one command:

```
source("<full pathname goes here>/exampleCommands.txt")
```

Appendix C shows an example workflow that produces pdfs of all the graphics and text files for all the tables in one folder.

References Cited

Baker, D.B., and Richards, R.P., 2002, Phosphorus Budgets and Riverine Phosphorus Export in Northwestern Ohio Watersheds: J. Environ. Qual., v. 31, p. 96–108.

Cleveland, W.S., 1979, Robust Locally Weighted Regression and Smoothing Scatterplots: Journal of the American Statistical Association, v. 74, no. 368, p. 829–836.

Cleveland, W.S., and Devlin, S.J., 1988, Locally Weighted Regression: An Approach to Regression Analysis by Local Fitting: Journal of the American Statistical Association, v. 83, no. 403, p. 596–610.

Cohn, T.A., Caulder, D.L., Gilroy, E.J., Zynjuk, L.D., and Summers, R.M., 1992, The validity of a simple statistical model for estimating fluvial constituent loads: An Empirical study involving nutrient loads entering Chesapeake Bay: Water Resources Research, v. 28, no. 9, p. 2353–2363.

Debrewer,, L., Ator, S., and Denver, J., 2008, Temporal Trends in Nitrate and Selected Pesticides in Mid-Atlantic Ground Water: J. Environ. Qual., v. 37, no. 5_Supplement, p. S–296–S–308.

Garrett, J.D., 2012, Concentrations, Loads, and Yields of Select Constituents from Major Tributaries of the Mississippi and Missouri Rivers in Iowa, Water Years 2004–2008:.

Geological Survey (U.S.), 1998, National Water Information System (NWIS): Fact Sheet, p. 1 sheet ([2] p.) : ill. (some col.) ; 28 cm. ill. (some col.) ;

Gordon, N.D., McMahon, T.A., and Finlayson, B.L., 1991, Stream hydrology: an introduction for ecologists.: John Wiley and Sons Ltd, New York, 429 p.

Helsel, D., and Hirsch, R., 2002, Statistical methods in water resources: US Geological Survey Techniques of Water Resources Investigations, book 4, chap:.

Hirsch, R.M., 2012, Flux of Nitrogen, Phosphorus, and Suspended Sediment from the Susquehanna River Basin to the Chesapeake Bay During Tropical Storm Lee, September 2011, as an Indicator of the Effects of Reservoir Sedimentation on Water Quality: USGS Scientific Investigations Report, US Department of the Interior, US Geological Survey, 17 p.

Hirsch, R.M., 2014, Large biases in regression-based constituent flux estimates: causes and diagnostic tools: Journal of the American Water Resources Association, v. In press.

Hirsch, R.M., Moyer, D.L., and Archfield, S.A., 2010, Weighted Regressions on Time, Discharge, and Season (WRTDS), with an Application to Chesapeake Bay River Inputs1: JAWRA Journal of the American Water Resources Association, v. 46, no. 5, p. 857–880.

Hirsch, R.M., Slack, J.R., and Smith, R.A., 1982, Techniques of trend analysis for monthly water quality data: Water resources research, v. 18, no. 1, p. 107–121.

Kalkhoff, S.J., 2013, Occurrence and transport of nutrients in the Missouri River Basin, April through September 2011, *in* U.S. Geological Survey Porfessional Paper, U.S. Geological Survey, p. 23.

Montgomery, D.C., Peck, E.A., and Vining, G.G., 2012, Introduction to linear regression analysis: Wiley.

Moyer, D., Hirsch, R., and Hyer, K., 2012, Comparison of two regression-based approaches for determining nutrient and sediment fluxes and trends in the Chesapeake Bay watershed: US Geological Survey Scientific Investigations Report 2012-5244, 118 p: Also available online at http://pubs. usgs. gov/sir/2012/5244/.

Murphy, J.C., Hirsch, R.M., and Sprague, L.A., 2014, Antecedent flow conditions and nitrate concentrations in the Mississippi River basin: Hydrology and Earth System Sciences, v. 18, no. 3, p. 967–979.

Peter Richards, R., Alameddine, I., David Allan, J., Baker, D.B., Bosch, N.S., Confesor, R., DePinto, J.V., Dolan, D.M., Reutter, J.M., and Scavia, D., 2012, "Nutrient Inputs to the Laurentian Great Lakes by Source and Watershed Estimated Using SPARROW Watershed Models" by Dale M. Robertson and David A. Saad2: JAWRA Journal of the American Water Resources Association.

Rice, K.C., and Hirsch, R.M., 2012, Spatial and Temporal Trends in Runoff at Long-term Streamgages Within and Near the Chesapeake Bay Watershed: US Geological Survey.

Richards, R.P., and Baker, D.B., 2002, Trends in Water Quality in LEASEQ Rivers and Streams (Northwestern Ohio), 1975–1995: J. Environ. Qual., v. 31, no. 1, p. 90–96.

Riggs, H.C., 1982, Low-flow investigations, *in* U.S. Geological Survey Techniques of Water-Resources Investigations, U.S. Geological Survey, p. 18.

Runkel, R., Crawford, C., and Cohn, TA, 2004, Load Estimator (LOADEST): A FORTRAN Program for Estimating Constituent Loads in Streams and Rivers, *in* US Geological Survey Techniques and Methods,.

Scott, J., Gellenbeck, D., Young, D., and Booth, N., 2008, U.S. federal water quality web service collaboration: United States Geological Survey,.

Stenback, G.A., Crumpton, W.G., Schilling, K.E., and Helmers, M.J., 2011, Rating curve estimation of nutrient loads in Iowa rivers: Journal of Hydrology, v. 396, no. 1, p. 158–169.

Tobin, J., 1958, Estimation of relationships for limited dependent variables: Econometrica: journal of the Econometric Society, p. 24–36.

Tukey, J.W., 1977, Exploratory data analysis: Reading, Ma, v. 231.

Appendix

Appendix A: dataRetrieval vignette

Appendix B: EGRET vignette

Appendix C: Batch workflows

These scripts are intended as examples of how a batch processing plan might be structured. They also provide a reference of common basic workflows that users might follow interactively.

```
library(dataRetrieval)
library(EGRET)

# list of sites
sites <- c("01491000", "11264500")
savePath <- "D:/LADData/RCode/Example1/"
fileNames <- rep(NA,length(sites))

for (i in 1:length(sites)){
  ############################
  # Gather discharge data:

  startDate <- "" #Gets earliest date
  endDate <- "2011-09-30"
  Daily <- getDVData(sites[i],"00060",startDate,endDate)

  # Gather sample data:
  parameter_cd<-"00631" #5 digit USGS code
  Sample <- getSampleData(sites[i],parameter_cd,startDate,endDate)

  # Gather site and parameter information:
  INFO<- getMetaData(sites[i],parameter_cd,interactive=FALSE)
  INFO$staAbbrev <- strsplit(INFO$station.nm," ")[[1]][1]
  INFO <- setPA()

  # Merge discharge with sample data:
  Sample <- mergeReport()
  ############################

  fileNames[i] <- paste(savePath, INFO$staAbbrev, ".",
                        INFO$constitAbbrev,".RData", sep = "")
  saveResults(savePath)
}

for (i in fileNames){

  load(i)

  pdf(paste(savePath,INFO$staAbbrev,
            "_FlowHistoryPlots.pdf",sep=""))
  ############################
  # Check flow history data:
  annualSeries <- makeAnnualSeries()
  plotFlowSingle(istat=7,qUnit="thousandCfs")
  plotSDLogQ()
  plotQTimeDaily(qLower=1,qUnit=3)
  plotFour(qUnit=3)
  plotFourStats(qUnit=3)
  ############################
  dev.off()
```

```
pdf(paste(savePath,INFO$staAbbrev,
          "_ConcHistoryPlots.pdf",sep=""))
############################
# Check sample data:
boxConcMonth()
boxQTwice()
plotConcTime()
plotConcQ()
multiPlotDataOverview()
############################
dev.off()

############################
# Run WRTDS model:
modelEstimation()
############################

pdf(paste(savePath,INFO$staAbbrev,
          "_WRTDS_Plots.pdf",sep=""))
  ############################
  #Check model results:

  plotConcTimeDaily()
  plotFluxTimeDaily()
  plotConcPred()
  plotFluxPred()
  plotResidPred()
  plotResidQ()
  plotResidTime()
  boxResidMonth()
  boxConcThree()

  #Explore trend results:
  plotConcHist()
  plotFluxHist()

  # Multi-line plots:
  date1 <- "2000-09-01"
  date2 <- "2005-09-01"
  date3 <- "2009-09-01"
  qBottom<-100
  qTop<-5000
  plotConcQSmooth(date1, date2, date3, qBottom, qTop,
                  concMax=2,qUnit=1)
  q1 <- 10
  q2 <- 25
  q3 <- 75
  centerDate <- "07-01"
  yearEnd <- 2010
  yearStart <- 2000
  plotConcTimeSmooth(q1, q2, q3, centerDate, yearStart, yearEnd)

  # Multi-plots:
  fluxBiasMulti()

  #Contour plots:
  clevel<-seq(0,2,0.5)
```

```
    maxDiff<-0.8

    plotContours(yearStart,yearEnd,qBottom,qTop,
                 contourLevels = clevel,qUnit=1)
    plotDiffContours(yearStart,yearEnd,
                     qBottom,qTop,maxDiff,qUnit=1)
  dev.off()

  concChange <- tableChangeSingle(returnDataFrame=TRUE,flux=FALSE)
  write.csv(concChange,file=paste(savePath,INFO$staAbbrev,
                                  "_concChange.csv",sep=""))
  fluxChange <- tableChangeSingle(returnDataFrame=TRUE,flux=TRUE)
  write.csv(fluxChange,file=paste(savePath,INFO$staAbbrev,
                                  "_fluxChange.csv",sep=""))

  sink(paste(savePath,INFO$staAbbrev,"_tableFlowChange.txt",sep=""))
  tableFlowChange(istat=1)
  sink()

  saveResults(savePath)

}
```